DEAN'S HANDBOOK OF ORGANIC CHEMISTRY

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PREFACE

The first edition of the *Handbook of Organic Chemistry* was edited by Professor John A. Dean. It appeared in 1987 and has served as a widely used and convenient reference work for more than 15 years. When Professor Dean asked if I would work with him to develop a second edition, I was pleased to do so. I felt that as valuable as the first edition was, it would be more broadly useful if it contained discussions of the data, the means by which the data were acquired, and perhaps even how the data are applied in modern science. We thus began the revision with enhanced usability as the foremost goal. Sadly, just as we were beginning the effort, Professor Dean passed away. He will be sorely missed.

In following the original plan, many figures, structures, discussions of the methods, and illustrations of the data have been incorporated. Some tables have been reorganized. In some cases tables have been printed twice; although they contain the same data, they are arranged by different criteria. The intent is to make the data easier for the researcher to access and use. Some Internet addresses that can serve as a supplementary resource are included. Despite the numerous additions, the volume remains compact and accessible.

As Professor Dean was not involved in producing this edition, I take responsibility for errors of fact or omission. I hope the volume is error-free, but I would appreciate being informed of any mistakes that are found. Finally, I wish to express my thanks to Mrs. Jolanta Pajewska, who helped in improving the manuscript and the proofreading.

GEORGE W. GOKEL

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SECTION 1

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1.2 SECTION 1

NOMENCLATURE OF ORGANIC COMPOUNDS

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

Hydrocarbons and Heterocycles

Alkanes. The saturated open-chain (acyclic) hydrocarbons (C_nH_{2n+2}) have names ending in -ane. The first four members have the trivial names *methane* (CH_4), *ethane* (CH_3CH_3 or C_2H_6), *propane* (C_3H_8), and *butane* (C_4H_{10}). For the remainder of the alkanes, the first portion of the name is derived from the Greek prefix (see Table 11.4) that cites the number of carbons in the alkane followed by -ane with elision of the terminal -a from the prefix, as shown in Table 1.1.

TABLE 1.1	Names of Straight-Cha	in Alkanes
-----------	-----------------------	------------

n^*	Name	n*	Name	n*	Name	n*	Name
1 2 3 4 5 6 7 8 9	Methane Ethane Propane Butane Pentane Hexane Heptane Octane Nonane†	11 12 13 14 15 16 17 18 19 20	Undecane‡ Dodecane Tridecane Tetradecane Pentadecane Hexadecane Heptadecane Octadecane Nonadecane Icosane8	21 22 23 30 31 32 40 50	Henicosane Docosane Tricosane Triacontane Hentriacontane Dotriacontane Tetracontane	60 70 80 90 100 110 120 121	Hexacontane Heptacontane Octacontane Nonacontane Hectane Decahectane Icosahectane Henicosahectane

^{*}n = total number of carbon atoms.

For branching compounds, the parent structure is the longest continuous chain present in the compound. Consider the compound to have been derived from this structure by replacement of hydrogen by various alkyl groups. Arabic number prefixes indicate the carbon to which the alkyl group is attached. Start numbering at whichever end of the parent structure that results in the lowest-numbered locants. The arabic prefixes are listed in numerical sequence, separated from each other by commas and from the remainder of the name by a hyphen.

If the same alkyl group occurs more than once as a side chain, this is indicated by the prefixes di-, tri-, tetra-, etc. Side chains are cited in alphabetical order (before insertion of any multiplying prefix). The name of a complex radical (side chain) is considered to begin with the first letter of its complete name. Where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest-numbered locant at the first cited point of difference in the radical. If two or more side chains are in equivalent positions, the one to be assigned the lowest-numbered locant is that cited first in the name. The complete expression for the side chain may be enclosed in parentheses for clarity or the carbon atoms in side chains may be indicated by primed locants.

[†] Formerly called enneane.

[‡] Formerly called hendecane.

[§] Formerly called eicosane.

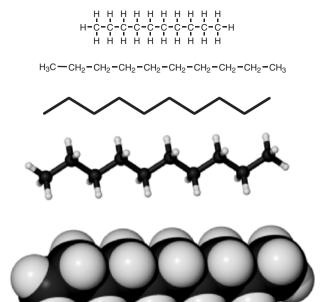


FIGURE 1.1 Projections for *n*-decane

If hydrocarbon chains of equal length are competing for selection as the parent, the choice goes in descending order to (1) the chain that has the greatest number of side chains, (2) the chain whose side chains have the lowest-numbered locants, (3) the chain having the greatest number of carbon atoms in the smaller side chains, or (4) the chain having the least-branched side chains.

These trivial names may be used for the unsubstituted hydrocarbons only:

Isobutane (CH₃)₂CHCH₃ Neopentane (CH₃)₄C Isopentane (CH₃)₂CHCH₂CH₃ Isohexane (CH₃)₂CHCH₂CH₂CH₃

Univalent radicals derived from saturated unbranched alkanes by removal of hydrogen from a terminal carbon atom are named by adding -yl in place of -ane to the stem name. Thus the alkane *ethane* becomes the radical *ethyl*. These exceptions are permitted for unsubstituted radicals only:

Note the usage of the prefixes iso-, neo-, *sec*-, and *tert*-, and note when italics are employed. Italicized prefixes are never involved in alphabetization, except among themselves; thus *sec*-butyl would precede isobutyl, isohexyl would precede isopropyl, and *sec*-butyl would precede *tert*-butyl.

Examples of alkane nomenclature are

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$$\overset{4}{C}H_{3} - \overset{2}{C}H_{2} - \overset{2}{C}H - \overset{1}{C}H_{3}$$
 2-Methylbutane (or the trivial name, isopentane)
$$\overset{4}{C}H_{3} + \overset{2}{C}H_{3}$$

$$\overset{5}{\text{C}}\text{H}_{3} - \overset{4}{\text{C}}\text{H}_{2} - \overset{3}{\text{C}}\text{H} - \text{CH}_{3} \\ \overset{1}{\text{C}}\text{H}_{2} - \overset{1}{\text{C}}\text{H}_{3}$$
 3-Methylpentane (not 2-ethylbutane)

5-Ethyl-2,2-dimethyloctane (note cited order)

$${\overset{8}{\text{C}}} {\overset{}{\text{H}}}_{3} - {\overset{7}{\text{C}}} {\overset{}{\text{H}}}_{2} - {\overset{6}{\text{C}}} {\overset{}{\text{H}}} - {\overset{5}{\text{C}}} {\overset{}{\text{H}}}_{2} - {\overset{3}{\text{C}}} {\overset{}{\text{H}}} - {\overset{2}{\text{C}}} {\overset{}{\text{H}}}_{2} - {\overset{1}{\text{C}}} {\overset{}{\text{H}}}_{3} \\ {\overset{1}{\text{C}}} {\overset{1}{\text{C}}} {\overset{1}{\text{H}}}_{3} - {\overset{1}{\text{C}}} {\overset{1}{\text{H}}}_{3}$$

3-Ethyl-6-methyloctane (note locants reversed)

$$\begin{matrix} \overset{\overset{\circ}{C}H_3}{\overset{\circ}{C}H_3} \\ CH_3 \overset{\overset{1}{-}\overset{1}{C}}{\overset{-}{C}CH_3} & CH_3 \\ \overset{\circ}{C}H_3 \overset{-}{\overset{\circ}{C}}H_2 \overset{-}{\overset{\circ}{C}}H_2 \overset{-}{\overset{\circ}{C}}H_2 \overset{-}{\overset{\circ}{C}}H \overset{-}{\overset{\circ}{C}}H_3 \\ CH_3 \overset{-}{\overset{-}{C}}{\overset{-}{C}CH_3} \\ CH_3 & \overset{\circ}{\overset{-}{C}}H_3 \end{matrix}$$

4,4-Bis(1,1-dimethylethyl)-2-methyloctane 4,4-Bis-1',1'-dimethylethyl-2-methyloctane 4,4-Bis(*tert*-butyl)-2-methyloctane

Bivalent radicals derived from saturated unbranched alkanes by removal of two hydrogen atoms are named as follows: (1) If both free bonds are on the same carbon atom, the ending -ane of the hydrocarbon is replaced with -ylidene. However, for the first member of the alkanes it is methylene rather than methylidene. Isopropylidene, *sec*-butylidene, and neopentylidene may be used for the unsubstituted group only. (2) If the two free bonds are on different carbon atoms, the straight-chain group terminating in these two carbon atoms is named by citing the number of methylene groups comprising the chain. Other carbons groups are named as substituents. Ethylene is used rather than dimethylene for the first member of the series, and propylene is retained for CH₃—CH—CH₂— (but trimethylene is —CH₂—CH₂—CH₂—).

Trivalent groups derived by the removal of three hydrogen atoms from the same carbon are named by replacing the ending -ane of the parent hydrocarbon with -ylidyne.

Alkenes and Alkynes. Each name of the corresponding saturated hydrocarbon is converted to the corresponding alkene by changing the ending -ane to -ene. For alkynes the ending is -yne. With more than one double (or triple) bond, the endings are -adiene, -atriene, etc. (or -adiyne, -atriyne, etc.). The position of the double (or triple) bond in the parent chain is indicated by a locant obtained by numbering from the end of the chain nearest the double (or triple) bond; thus CH₃CH₂CH=CH₂ is 1-butene and CH₃C≡CCH₃ is 2-butyne.

For multiple unsaturated bonds, the chain is so numbered as to give the lowest possible locants to the unsaturated bonds. When there is a choice in numbering, the double

bonds are given the lowest locants, and the alkene is cited before the alkyne where both occur in the name. Examples:

$$\begin{array}{lll} CH_3CH_2CH_2CH=CH-CH=CH_2 & 1,3\text{-Octadiene} \\ CH_2=CHC\equiv CCH=CH_2 & 1,5\text{-Hexadiene-3-yne} \\ CH_3CH=CHCH_2C\equiv CH & 4\text{-Hexen-1-yne} \\ CH\equiv CCH_2CH=CH_2 & 1\text{-Penten-4-yne} \end{array}$$

Unsaturated branched acyclic hydrocarbons are named as derivatives of the chain that contains the maximum number of double and/or triple bonds. When a choice exists, priority goes in sequence to (1) the chain with the greatest number of carbon atoms and (2) the chain containing the maximum number of double bonds.

These nonsystematic names are retained:

Ethylene
$$CH_2 = CH_2$$

Allene $CH_2 = C = CH_2$
Acetylene $HC = CH$

An example of nomenclature for alkenes and alkynes is

$$\begin{array}{c} CH_2-CH_2-CH_3 \\ H\overset{6}{C}=\overset{5}{C}-\overset{1}{C}=\overset{3}{C}-\overset{2}{C}H=\overset{1}{C}H_2 \\ CH=CH_2 \end{array} \quad \text{4-Propyl-3-vinyl-1,3-hexadien-5-yne}$$

Univalent radicals have the endings -enyl, -ynyl, -dienyl, -diynyl, etc. When necessary, the positions of the double and triple bonds are indicated by locants, with the carbon atom with the free valence numbered as 1. Examples:

$$\begin{array}{lll} CH_2 \!\!=\!\! CH \!\!-\!\! CH_2 \!\!-\!\! & 2\text{-Propenyl} \\ CH_3 \!\!-\!\! C \!\!\equiv\!\! C \!\!-\!\! & 1\text{-Propynyl} \\ CH_3 \!\!-\!\! C \!\!\equiv\!\! C \!\!-\!\! CH_2 \!\!CH \!\!=\!\! CH_2 \!\!-\!\! & 1\text{-Hexen-4-ynyl} \end{array}$$

These names are retained:

Vinyl (for ethenyl)
$$CH_2$$
= CH — Allyl (for 2-propenyl) CH_2 = CH — CH_2 — Isopropenyl (for 1-methylvinyl but for unsubstituted radical only) CH_2 = $C(CH_3)$ —

Should there be a choice for the fundamental straight chain of a radical, that chain is selected which contains (1) the maximum number of double and triple bonds, (2) the largest number of carbon atoms, and (3) the largest number of double bonds. These are in descending priority.

Bivalent radicals derived from unbranched alkenes, alkadienes, and alkynes by removing a hydrogen atom from each of the terminal carbon atoms are named by replacing the endings -ene, -diene, and -yne by -enylene, -dienylene, and -ynylene, respectively. Positions of double and triple bonds are indicated by numbers when necessary. The name *vinylene* instead of ethenylene is retained for —CH—CH—.

Monocyclic Aliphatic Hydrocarbons. Monocyclic aliphatic hydrocarbons (with no side chains) are named by prefixing cyclo- to the name of the corresponding open-chain hydrocarbon having the same number of carbon atoms as the ring. Radicals are formed as with the alkanes, alkenes, and alkynes. Examples:

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For convenience, aliphatic rings are often represented by simple geometric figures: a triangle for cyclopropane, a square for cyclobutane, a pentagon for cyclopentane, a hexagon (as illustrated) for cyclohexane, etc. It is understood that two hydrogen atoms are located at each corner of the figure unless some other group is indicated for one or both.

Monocyclic Aromatic Compounds. Except for six retained names, all monocyclic substituted aromatic hydrocarbons are named systematically as derivatives of benzene. Moreover, if the substituent introduced into a compound with a retained trivial name is identical with one already present in that compound, the compound is named as a derivative of benzene. These names are retained:

The position of substituents is indicated by numbers, with the lowest locant possible given to substituents. When a name is based on a recognized trivial name, priority for lowest-numbered locants is given to substituents implied by the trivial name. When only two substituents are present on a benzene ring, their position may be indicated by *o-* (*ortho-*), *m-* (*meta-*), and *p-* (*para-*) (and alphabetized in the order given) used in place of 1,2-, 1,3-, and 1,4-, respectively.

Radicals derived from monocyclic substituted aromatic hydrocarbons and having the free valence at a ring atom (numbered 1) are named phenyl (for benzene as parent, since benzyl is used for the radical $C_6H_5CH_2$ —), cumenyl, mesityl, tolyl, and xylyl. All other radicals are named as substituted phenyl radicals. For radicals having a single free valence in the side chain, these trivial names are retained:

Benzyl $C_6H_5CH_2$ — Phenethyl $C_6H_5CH_2CH_2$ —
Benzhydryl (alternative to diphenylmethyl) $(C_6H_5)_2CH$ — Trityl $(C_6H_5)_3C$ —
Cinnamyl C_6H_5CH =CH- CH_2 —

Otherwise, radicals having the free valence(s) in the side chain are named in accordance with the rules for alkanes, alkenes, or alkynes.

The name *phenylene* (o-, m-, or p-) is retained for the radical $-C_6H_4$ —. Bivalent radicals formed from substituted benzene derivatives and having the free valences at ring atoms are named as substituted phenylene radicals, with the carbon atoms having the free valences being numbered 1,2-, 1,3-, or 1,4-, as appropriate.

Radicals having three or more free valences are named by adding the suffixes -triyl, -tetrayl, etc. to the systematic name of the corresponding hydrocarbon.

Fused Polycyclic Hydrocarbons. The names of polycyclic hydrocarbons containing the maximum number of conjugated double bonds end in -ene. Here the ending does not denote one double bond. Names of hydrocarbons containing five or more fixed benzene rings in a linear arrangement are formed from a numerical prefix (see Table 11.4) followed by -acene. A partial list of the names of polycyclic hydrocarbons is given in Table 1.2. Many names are trivial.

Numbering of each ring system is fixed, as shown in Table 1.2, but it follows a systematic pattern. The individual rings of each system are oriented so that the greatest number of rings are (1) in a horizontal row and (2) the maximum number of rings are above and to the right (upper-right quadrant) of the horizontal row. When two orientations meet these requirements, the one is chosen that has the fewest rings in the lower-left quadrant. Numbering proceeds in a clockwise direction, commencing with the carbon atom not engaged in ring fusion that lies in the most counterclockwise position of the uppermost ring (upper-right quadrant); omit atoms common to two or more rings. Atoms common to two or more rings are designated by adding lowercase roman letters to the number of the position immediately preceding. Interior atoms follow the highest number, taking a clockwise sequence wherever there is a choice. Anthracene and phenanthrene are two exceptions to the rule on numbering. Two examples of numbering follow:

When a ring system with the maximum number of conjugated double bonds can exist in two or more forms differing only in the position of an "extra" hydrogen atom, the name can be made specific by indicating the position of the extra hydrogen(s). The compound name is modified with a locant followed by an italic capital H for each of these hydrogen atoms. Carbon atoms that carry an indicated hydrogen atom are numbered as low as possible. For example, 1H-indene is illustrated in Table 1.2; 2H-indene would be

Names of polycyclic hydrocarbons with less than the maximum number of noncumulative double bonds are formed from a prefix dihydro-, tetrahydro-, etc., followed by the

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name of the corresponding unreduced hydrocarbon. The prefix perhydro- signifies full hydrogenation. For example, 1,2-dihydronaphthalene is

$$H_{2}$$
 H_{2}
 H_{3}

TABLE 1.2 Fused Polycyclic Hydrocarbons

Listed in order of increasing priority for selection as parent compound

Asterisk after a compound denotes exception to systematic numbering.

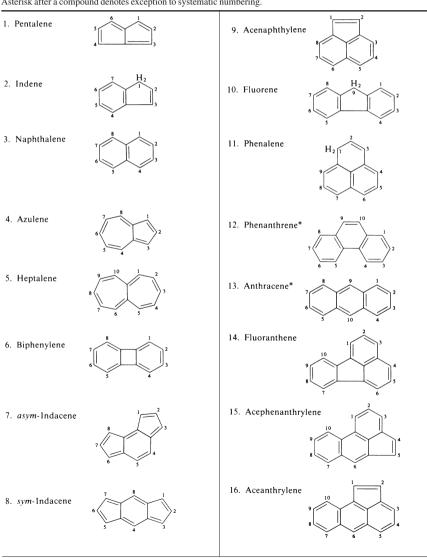


TABLE 1.2 Fused Polycyclic Hydrocarbons (continued)

Listed in order of increasing priority for selection as parent compound

Asterisk after a compound denotes exception to systematic numbering.

Examples of retained names and their structures are as follows:

Polycyclic compounds in which two rings have two atoms in common or in which one ring contains two atoms in common with each of two or more rings of a contiguous series of rings and which contain at least two rings of five or more members with the maximum number of noncumulative double bonds and which have no accepted trivial name (Table 1.2) are named by prefixing to the name of the parent ring or ring system designations of the other components. The parent name should contain as many rings as possible (provided it has a trivial name) and should occur as far as possible from the beginning of the list in Table 1.2. Furthermore, the attached component(s) should be as simple as possible. For example, one writes dibenzo phenanthrene and not naphthophenanthrene because the attached component benzo- is simpler than naphtho-. Prefixes designating attached components are formed by changing the ending -ene into -eno-; for example, indeno- from

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indene. Multiple prefixes are arranged in alphabetical order. Several abbreviated prefixes are recognized; the parent is given in parentheses:

Acenaphtho- (acenaphthylene) Naphtho- (naphthalene)
Anthra- (anthracene) Perylo- (perylene)
Benzo- (benzene) Phenanthro- (phenanthrene)

For monocyclic prefixes other than benzo-, the following names are recognized, each to represent the form with the maximum number of noncumulative double bonds: cyclopenta-, cyclopenta-, cyclopenta-, cyclopenta-, etc.

Isomers are distinguished by lettering the peripheral sides of the parent beginning with a for the side 1,2-, and so on, lettering every side around the periphery. If necessary for clarity, the numbers of the attached position (1,2-, for example) of the substituent ring are also denoted. The prefixes are cited in alphabetical order. The numbers and letters are enclosed in square brackets and placed immediately after the designation of the attached component. Examples are

Bridged Hydrocarbons. Saturated alicyclic hydrocarbon systems consisting of two rings that have two or more atoms in common take the name of the open-chain hydrocarbon containing the same total number of carbon atoms and are preceded by the prefix bicyclo-. The system is numbered commencing with one of the bridgeheads, numbering proceeding by the longest possible path to the second bridgehead. Numbering is then continued from this atom by the longer remaining unnumbered path back to the first bridgehead and is completed by the shortest path from the atom next to the first bridgehead. When a choice in numbering exists, unsaturation is given the lowest numbers. The number of carbon atoms in each of the bridges connecting the bridgeheads is indicated in brackets in descending order. Examples are

Hydrocarbon Ring Assemblies. Assemblies are two or more cyclic systems, either single rings or fused systems, that are joined directly to each other by double or single bonds. For identical systems naming may proceed (1) by placing the prefix bi- before the name of the corresponding radical or (2) for systems joined through a single bond, by placing the prefix bi- before the name of the corresponding hydrocarbon. In each case, the numbering of the assembly is that of the corresponding radical or hydrocarbon, one system being assigned unprimed numbers and the other primed numbers. The points of attachment

are indicated by placing the appropriate locants before the name; an unprimed number is considered lower than the same number primed. The name *biphenyl* is used for the assembly consisting of two benzene rings. Examples are

1,1'-Bicyclopropyl or 1,1'-bicyclopropane

2-Ethyl-2'-propylbiphenyl

For nonidentical ring systems, one ring system is selected as the parent and the other systems are considered as substituents and are arranged in alphabetical order. The parent ring system is assigned unprimed numbers. The parent is chosen by considering the following characteristics in turn until a decision is reached: (1) the system containing the larger number of rings, (2) the system containing the larger ring, (3) the system in the lowest state of hydrogenation, and (4) the highest-order number of ring systems set forth in Table 1.2. Examples are given, with the deciding priority given in parentheses preceding the name:

- (1) 2-Phenylnaphthalene
- (2) and (4) 2-(2'-Naphthyl)azulene
- (3) Cyclohexylbenzene

Radicals from Ring Systems. Univalent substituent groups derived from polycyclic hydrocarbons are named by changing the final e of the hydrocarbon name to -yl. The carbon atoms having free valences are given locants as low as possible consistent with the fixed numbering of the hydrocarbon. Exceptions are naphthyl (instead of naphthalenyl), anthryl (for anthracenyl), and phenanthryl (for phenanthrenyl). However, these abbreviated forms are used only for the simple ring systems. Substituting groups derived from fused derivatives of these ring systems are named systematically. Substituting groups having two or more free bonds are named as described in Monocyclic Aliphatic Hydrocarbons on p. 1.5.

Cyclic Hydrocarbons with Side Chains. Hydrocarbons composed of cyclic and aliphatic chains are named in a manner that is the simplest permissible or the most appropriate for the chemical intent. Hydrocarbons containing several chains attached to one cyclic nucleus are generally named as derivatives of the cyclic compound, and compounds containing several side chains and/or cyclic radicals attached to one chain are named as derivatives of the acyclic compound. Examples are

2-Ethyl-1-methylnaphthalene Diphenylmethane

1,5-Diphenylpentane 2,3-Dimethyl-1-phenyl-1-hexene

Recognized trivial names for composite radicals are used if they lead to simplifications in naming. Examples are

1-Benzylnaphthalene 1,2,4-Tris(3-*p*-tolylpropyl)benzene

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Fulvene, for methylenecyclopentadiene, and stilbene, for 1,2-diphenylethylene, are trival names that are retained.

Heterocyclic Systems. Heterocyclic compounds can be named by relating them to the corresponding carbocyclic ring systems by using replacement nomenclature. Heteroatoms are denoted by prefixes ending in -a, as shown in Table 1.3. If two or more replacement prefixes are required in a single name, they are cited in the order of their listing in the table. The lowest possible numbers consistent with the numbering of the corresponding carbocyclic system are assigned to the heteroatoms and then to carbon atoms bearing double

 TABLE 1.3
 Specialist Nomenclature for Heterocyclic Systems

Heterocyclic atoms are listed in decreasing order of priority

Element	Valence	Prefix	Element	Valence	Prefix
Oxygen Sulfur Selenium Tellurium Nitrogen Phosphorus Arsenic	2 2 2 2 2 3 3 3	Oxa- Thia- Selena- Tellura- Aza- Phospha-* Arsa-*	Antimony Bismuth Silicon Germanium Tin Lead Boron Mercury	3 3 4 4 4 4 3 2	Stiba-* Bisma- Sila- Germa- Stanna- Plumba- Bora- Mercura-

^{*} When immediately followed by -in or -ine, phospha- should be replaced by phosphor-, arsa- by arsen-, and stiba- by antimon-. The saturated six-membered rings corresponding to phosphorin and arsenin are named *phosphorinane* and *arsenane*. A further exception is the replacement of borin by borinane.

TABLE 1.4 Suffixes for Specialist Nomenclature of Heterocyclic Systems

Number of	Rings containing	g nitrogen	Rings containing no nitrogen		
members	Unsaturation*	Saturation	Unsaturation*	Saturation	
3	-irine	-iridine	-irene	-irane	
4	-ete	-etidine	-ete	-etane	
5	-ole	-olidine	-ole	-olane	
6	-ine†	‡	-in	-ane§	
7	-epine	‡	-epin	-epane	
8	-ocine	‡	-ocin	-ocane	
9	-onine	‡	-onin	-onane	
10	-ecine	‡	-ecin	-ecane	

^{*} Unsaturation corresponding to the maximum number of noncumulative double bonds. Heteroatoms have the normal valences given in Table 1.3.

[†] For phosphorus, arsenic, antimony, and boron, see the special provisions in Table 1.3.

[‡] Expressed by prefixing perhydro- to the name of the corresponding unsaturated compound.

[§] Not applicable to silicon, germanium, tin, and lead; perhydro- is prefixed to the name of the corresponding
unsaturated compound.

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names Listed in order of increasing priority as senior ring system

Asterisk after a compound denotes exception to systematic numbering.

			1		
Structure	Parent name	Radical name	Structure	Parent name	Radical name
5 S 2	Thiophene	Thienyl	5 CH ₂	2 <i>H</i> -Pyrrole	2 <i>H</i> -Pyrrolyl
8 S S	2 3		H 5 N 1 2	Pyrrole	Pyrrolyl
6 \$	Thianthrene	Thianthrenyl		Imidazole	Imidazolyl
5 O 2	Furan	Furyl	H N 5 N 2	Pyrazole	Pyrazolyl
6 CH ₂	Pyran (2 <i>H</i> -shown)	Pyranyl	1 S N 2	Isothiazole	Isothiazolyl
6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Isobenzofuran) ²	Isobenzo- furanyl	5 N 2	Isoxazole	Isoxazolyl
7 0 2 0 2 6 5 4	CH ₂		6 N 2 3	Pyridine	Pyridyl
8 H ₂ C	Chromene (2 <i>H</i> -shown)	Chromenyl	6 N 2 3	Pyrazine	Pyrazinyl
6 S O	3 Xanthene*	Xanthenyl		Pyrimidine	Pyrimidinyl
8 S S S S S S S S S S S S S S S S S S S	2 3		1 N 2 1 N 2	Pyridazine	Pyridazinyl
	Phenoxathiin	Phenoxa- thiinyl	5 4 113		

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TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (continued) Listed in order of increasing priority as senior ring system

Asterisk after a compound denotes exception to systematic numbering.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Indolizine	Indolizinyl	$\begin{bmatrix} 7 & & & & & & \\ & & & & & & \\ & & & & &$	Phthalazine	Phthalazinyl
6 2NH	Isoindole	Isoindolyl	7 N N 2 3	Naphthyri- dine (1,8-shown)	Naphthyri- dinyl
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 <i>H</i> -Indole	3 <i>H</i> -Indolyl	5 4 7 N 3	Quinoxaline	Quinoxalinyl
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Indole	Indolyl	5 4 N	Quinazoline	Quinazolinyl
6 H N 1 N 2	<i>H</i> -Indazole	l <i>H-</i> Indazolyl	5 4 7 N N S	2 Cinnoline	Cinnolinyl
1 N 1 N 8	Purine*	Purinyl	7 8 1 N 1 N 1 N 1 N 1 N 1 N 1 N 1 N 1 N 1	Pteridine	Pteridinyl
$ \begin{array}{c} 8 \\ 7 \\ 6 \end{array} $ $ \begin{array}{c} 1 \\ 7 \\ 6 \end{array} $ $ \begin{array}{c} 4 \\ C \\ H_2 \end{array} $	4 <i>H</i> -Quin- olizine	4 <i>H</i> -Quin- olizinyl	8 N y	2 3	
7 8 1 N	² Isoquinoline	Isoquinolyl	. н	4αH- Carbazole*	4α <i>H</i> - Carbazolyl
3 4 N 3	Quinoline	Quinolyl	7 6 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	2 3	
5 4				Carbazole*	Carbazolyl

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (continued) Listed in order of increasing priority as senior ring system

Asterisk after a compound denotes exception to systematic numbering.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
8 H N 9	N ²		8 9 10 N	2 3	
	β -Carboline	β -Carbolinyl		Phenazine	Phenazinyl
9 10 1	2 3 4 2 N_5 Phenanthri-	Phenanthri-	8 AS N 5	1 2 3	
	dine	dinyl		Phenarsazine	Phenarsazinyl
7 8 9 9 6 5 N	1 2 3 Acridine*	Acridinyl	8 H N 10 7 S S S S	2 3	
HN_1	Perimidine	Perimidinyl		Phenothiazine	Phenothiazinyl
9 8 7 6	5		5 N O N 2	Furazan	Furazanyl
9 N N N N N N N N N N N N N N N N N N N	henanthroline	Phenanthrolinyl	8 HN 10 O S	¹ / ₃	
	(1,10-shown)			Phenoxazine	Penoxazinyl

or triple bonds. Locants are cited immediately preceding the prefixes or suffixes to which they refer. Multiplicity of the same heteroatom is indicated by the appropriate prefix in the series: di-, tri-, tetra-, penta-, hexa-, etc.

If the corresponding carbocyclic system is partially or completely hydrogenated, the additional hydrogen is cited using the appropriate H- or hydro- prefixes. A trivial name from Tables 1.5 and 1.6, if available, along with the state of hydrogenation may be used. In the specialist nomenclature for heterocyclic systems, the prefix or prefixes from

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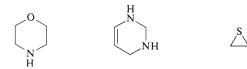
TABLE 1.6 Trivial Names for Heterocyclic Systems that are Not Recommended for Use in Fusion Names

Listed in order of increasing priority

Structure	Parent name	Radical name	Structure	Parent name	Radical name
7 6 5	O ²		1 H N 5 NH 2	Pyrazoline (3-shown*)	Pyrazolinyl
7 6	Isochroman	Isochromanyl	H N 2 5 4 3	Piperidine	Piperidyl†
5	Chroman	Chromanyl	6 H N 2 N N N N N N N N N N N N N N N N N	Piperazine	Piperazinyl
5 N 2	Pyrrolidine	Pyrrolidinyl	5 4 3 H		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Pyrroline (2-shown*)	Pyrrolinyl	6 1 H N	⟩² Indoline	Indolinyl
5 NH 3	Imidazolidine	Imidazolidinyl	6 7 1 2 5 4 3	NH Isoindoline	Isoindolinyl
5 N 2 N 3	Imidazoline (2-shown*)	Imidazolinyl	8 - N ¹	y 2	·
1 H N 1 N 1 NH	₂ Pyrazolidine	Pyrazolidinyl	O 2 3 N 3	Quinuclidine Morpholine	Quinuclidinyl Morpholinyl‡
	~ 61 11 1 1		H		

^{*} Denotes position of double bond. † For 1-piperidyl, use piperidino. ‡ For 4-morpholinyl, use morpholino.

Table 1.3 are combined with the appropriate stem from Table 1.4, eliding an -a where necessary. Examples of acceptable usage, including (1) replacement and (2) specialist nomenclature, are



- (1) 1-Oxa-4-azacyclohexane
- (2) 1,4-Oxazoline Morpholine
- (1) 1,3-Diazacyclohex-5-ene
- (2) 1,2,3,4-Tetrahydro-1,3-diazine
- (1) Thiacyclopropane
- (2) Thiirane Ethylene sulfide

Radicals derived from heterocyclic compounds by removal of hydrogen from a ring are named by adding -yl to the names of the parent compounds (with elision of the final e, if present). These exceptions are retained:

Furyl (from furan) Furfuryl (for 2-furylmethyl)

Pyridyl (from pyridine) Furfurylidene (for 2-furylmethylene)

Piperidyl (from piperidine) Thienyl (from thiophene)

Quinolyl (from quinoline) Thenylidyne (for thienylmethylidyne)
Isoquinolyl Furfurylidyne (for 2-furylmethylidyne)

Thenylidene (for thienylmethylene) Thenyl (for thienylmethyl)

Also, piperidino- and morpholino- are preferred to 1-piperidyl- and 4-morpholinyl-, respectively.

If there is a choice among heterocyclic systems, the parent compound is decided in the following order of preference:

- 1. A nitrogen-containing component
- ${\bf 2.}$ A component containing a heteroatom, in the absence of nitrogen, as high as possible in Table 1.3
- 3. A component containing the greatest number of rings
- 4. A component containing the largest possible individual ring
- 5. A component containing the greatest number of heteroatoms of any kind
- **6.** A component containing the greatest variety of heteroatoms
- 7. A component containing the greatest number of heteroatoms first listed in Table 1.3

If there is a choice between components of the same size containing the same number and kind of heteroatoms, choose as the base component that one with the lower numbers for the heteroatoms before fusion. When a fusion position is occupied by a heteroatom, the names of the component rings to be fused are selected to contain the heteroatom.

Common Names of Heterocycles Used Broadly in Biology. The naming of heterocycles by systematic methods is important but cumbersome for designating some of the most commonly occurring heterocycles. In particular, the bases that occur in ribonucleic acids (RNA) and deoxyribonucleic acids (DNA) have specific substitution patterns. Because they occur so commonly, they have been given trivial names that are invariably used when discussed or named in the biological literature.

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Base pairing is the most common (Watson-Crick) arrangement.

The individual elements of RNA and DNA chains.

FIGURE 1.2 Base pairing in the most common (Watson–Crick) arrangement. The individual elements of RNA and DNA chains are shown in the lower panel of the figure. Hollow arrows indicate the points at which the 5'-hydroxyl group is esterified to the 3'-phosphate group to form the so-called "sugar–phosphate" backbone. Note the hydroxyl group (arrow) that is present on ribose but missing in deoxyribose.

The structural frameworks of DNA and RNA are organized by hydrogen bond formation between pairs of purine and pyrimidine bases. The pyrimidines are shown near the end of Table 1.5. Cytosine (C) and thymine (T) occur in DNA and form hydrogen-bonded pairs with the purines guanine (G) and adenine (A), respectively. The base pairs are abbreviated AT and GC, sometimes with dotted lines connecting them. The AT pair is held together by two hydrogen bonds and may be represented in shorthand as A::T. Three H-bonds hold together guanine and cytosine, giving G:::C. The so-called Watson–Crick base pairing is shown in Figure 1.2. In RNA, uracil replaces thymine but pairing still occurs with adenine to give A::U.

An alternative form of hydrogen bonding between base pairs is designated "Hoogsteen." This type of bonding cannot readily occur in nature because the purine and pyrimidine bases are constrained to long chains that must interact at numerous points.

Functionalized Compounds

There are several types of nomenclature systems that are recognized. Which type to use is sometimes obvious from the nature of the compound. Substitutive nomenclature, in general, is preferred because of its broad applicability, but radicofunctional, additive, and replacement nomenclature systems are convenient in certain situations.

Substitutive Nomenclature. The first step is to determine the kind of characteristic (functional) group for use as the principal group of the parent compound. A characteristic group is a recognized combination of atoms that confers characteristic chemical properties on the molecule in which it occurs. Carbon-to-carbon unsaturation and heteroatoms in rings are considered nonfunctional for nomenclature purposes.

Substitution means the replacement of one or more hydrogen atoms in a given compound by some other kind of atom or group of atoms, functional or nonfunctional. In substitutive nomenclature, each substituent is cited as either a prefix or a suffix to the name of the parent (or substituting radical) to which it is attached; the latter is denoted the parent compound (or parent group if a radical).

In Table 1.7 are listed the general classes of compounds in descending order of preference for citation as suffixes, that is, as the parent or characteristic compound. When oxygen is

TABLE 1.7 Characteristic Groups for Substitutive Nomenclature

Listed in order of decreasing priority for citation as principal group or parent name

Class	Formula*	Prefix	Suffix
1. Cations	H_4N^+ H_3O^+ H_3S^+ H_3Se^+ H_2Cl^+ H_2Br^+ H_2I^+	-onio- Ammonio- Oxonio- Sulfonio- Selenonio- Chloronio- Bromonio- Iodonio-	-onium -ammonium -oxonium -sulfonium -selenonium -chloronium -bromonium -iodonium
2. Acids Carboxylic Sulfonic Sulfinic	$-COOH$ $-(C)OOH$ $-C(=O)OOH$ $-(C=O)OOH$ $-SO_3H$ $-SO_2H$	Carboxy- Sulfo- Sulfino-	-carboxylic acid -oic acid -peroxy···carboxylic acid -peroxy···oic acid -sulfonic acid -sulfinic acid
Sulfenic Salts	—SOH —COOM —(C)OOM —SO ₃ M —SO ₂ M —SOM	Sulfeno-	-sulfenic acid Metal ··· carboxylate Metal ··· oate Metal ··· sulfonate Metal ··· sulfinate Metal ··· sulfinate Metal ··· sulfenate
3. Derivatives of acids	-C(=0)OC(=0)-		aarhayydia anhydeida
Anhydrides Esters Acid halides Amides	C(=0)OC(=0)- -(C=0)O(C=0)- COOR C(OOR) CO-halogen CO-NH ₂ (C)O-NH ₂	R-oxycarbonyl- Haloformyl Carbamoyl-	-carboxylic anhydride -oic anhydride R···carboxylate R···oate -carbonyl halide -carboxamide -amide

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TABLE 1.7 Characteristic Groups for Substitutive Nomenclature (*continued*) *Listed in order of decreasing priority for citation as principal group or parent name*

Class	Formula*	Prefix	Suffix
Hydrazides	—CO—NHNH ₂ —(CO)—NHNH ₂	Carbonyl-hydrazino-	-carbohydrazide -ohydrazide
Imides Amidines	$-CO - NH - CO - C(=NH) - NH_2 - (C=NH) - NH_2$	R-imido- Amidino-	-carboximide -carboxamidine -amidine
4. Nitrile (cyanide)	—CN —(C)N	Cyano-	-carbonitrile -nitrile
5. Aldehydes	—CHO —(C=O)H (then their analogs and	Formyl- Oxo- d derivatives)	-carbaldehyde -al
6. Ketones	>(C=O) (then their analogs and	Oxo- d derivatives)	-one
7. Alcohols (and phenols)	—ОН	Hydroxy-	-ol
Thiols	—SH	Mercapto-	-thiol
8. Hydroperoxides	—О—ОН	Hydroperoxy-	
9. Amines Imines Hydrazines	$-NH_2$ $=NH$ $-NHNH_2$	Amino- Imino- Hydrazino-	-amine -imine -hydrazine
10. Ethers Sulfides	—OR —SR	R-oxy- R-thio-	
11. Peroxides	-O-OR	R-dioxy-	

^{*} Carbon atoms enclosed in parentheses are included in the name of the parent compound and not in the suffix or prefix.

replaced by sulfur, selenium, or tellurium, the priority for these elements is in the descending order listed. The higher valence states of each element are listed before considering the successive lower valence states. Derivative groups have priority for citation as principal group after the respective parents of their general class.

In Table 1.8 are listed characteristic groups that are cited only as prefixes (never as suffixes) in substitutive nomenclature. The order of listing has no significance for nomenclature purposes.

Systematic names formed by applying the principles of substitutive nomenclature are single words except for compounds named as acids. First one selects the parent compound, and thus the suffix, from the characteristic group listed earliest in Table 1.7. All remaining functional groups are handled as prefixes that precede, in alphabetical order, the parent name. Two examples may be helpful:

$$CH_3$$
 0
 $C-O-C_2H_5$ O
 $BrCH_2-CH_2-C-CH_2OH$
 OCH_3
 $Structure 1$ $Structure 2$

Characteristic group	Prefix	Characteristic group	Prefix
—Br	Bromo-	—IX ₂	X may be halogen or a radical; dihalogenoiodo-or diacetoxyiodo-, e.g., —ICl ₂ is dichloroido-
—Cl	Chloro-		_
—ClO	Chlorosyl-		
-ClO ₂	Chloryl-	=N⊕=N⊖	Diazo-
-ClO ₃	Perchloryl-	$-N_3, -N=N^{\oplus}=N^{\ominus}$	Azido-
—F	Fluoro-	-N=0	Nitroso-
—I	Iodo-	$-N = 0$ $-NO_{2}, -N = 0$	Nitro-
-IO	Iodosyl-	OH U	
		=N [⊕] <	aci-Nitro-
$-IO_2$	Iodyl*	—OR ^{`O} ⊜	R-oxy-; alkoxy- or aryloxy-
$-I(OH)_2$	Dihydroxyiodo-	—SR	R-thio-; alkylthio- or arylthio-
. 72		—SeR (—TeR)	R-seleno- (R-telluro-)

TABLE 1.8 Characteristic Groups Cited Only as Prefixes in Substitutive Nomenclature

Structure 1 contains an ester group and an ether group. Since the ester group has higher priority, the name is ethyl 2-methoxy-6-methyl-3-cyclohexene-1-carboxylate. Structure 2 contains a carbonyl group, an hydroxy group, and a bromo group. The latter is never a suffix. Between the other two, the carbonyl group has higher priority, the parent has -one as suffix, and the name is 4-bromo-1-hydroxy-2-butanone.

Selection of the principal alicyclic chain or ring system is governed by the following selection rules:

- 1. For purely alicyclic compounds, the selection process proceeds successively until a decision is reached: (a) the maximum number of substituents corresponding to the characteristic group cited earliest in Table 1.7, (b) the maximum number of double and triple bonds considered together, (c) the maximum length of the chain, and (d) the maximum number of double bonds. Additional criteria, if needed for complicated compounds, are given in the IUPAC nomenclature rules.
- 2. If the characteristic group occurs only in a chain that carries a cyclic substituent, the compound is named as an aliphatic compound into which the cyclic component is substituted; a radical prefix is used to denote the cyclic component. This chain need not be the longest chain.
- 3. If the characteristic group occurs in more than one carbon chain and the chains are not directly attached to one another, then the chain chosen as parent should carry the largest number of the characteristic group. If necessary, the selection is continued as in rule 1.
- **4.** If the characteristic group occurs only in one cyclic system, that system is chosen as the parent.
- 5. If the characteristic group occurs in more than one cyclic system, that system is chosen as parent which (a) carries the largest number of the principal group or, failing to reach a decision, (b) is the senior ring system.
- 6. If the characteristic group occurs both in a chain and in a cyclic system, the parent is that portion in which the principal group occurs in largest number. If the numbers are the same, that portion is chosen which is considered to be the most important or is the senior ring system.

^{*} Formerly iodoxy-.

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- 7. When a substituent is itself substituted, all the subsidiary substituents are named as prefixes and the entire assembly is regarded as a parent radical.
- 8. The seniority of ring systems is ascertained by applying the following rules successively until a decision is reached: (a) all heterocycles are senior to all carbocycles, (b) for heterocycles, the preference follows the decision process described under "Heterocyclic Systems," page 1–12, (c) the largest number of rings, (d) the largest individual ring at the first point of difference, (e) the largest number of atoms in common among rings, (f) the lowest letters in the expression for ring functions, (g) the lowest numbers at the first point of difference in the expression for ring junctions, (h) the lowest state of hydrogenation, (i) the lowest-numbered locant for indicated hydrogen, (j) the lowest-numbered locant for an attached group expressed as a suffix, (l) the maximum number of substituents cited as prefixes, (m) the lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order independent of their nature, and (n) the lowest-numbered locant for the substituent named as prefix which is cited first in the name.

Numbering of Compounds. If the rules for aliphatic chains and ring systems leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest-numbered locants to these structural factors, if present, considered successively in the order listed below until a decision is reached. Characteristic groups take precedence over multiple bonds.

- 1. Indicated hydrogen, whether cited in the name or omitted as being conventional.
- 2. Characteristic groups named as suffix following the ranking order of Table 1.7.
- 3. Multiple bonds in acyclic compounds; in bicycloalkanes, tricycloalkanes, and polycycloalkanes, double bonds having priority over triple bonds; and in heterocyclic systems whose names end in -etine, -oline, or -olene.
- **4.** The lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order.
- 5. The lowest locant for that substituent named as prefix which is cited first in the name.

For cyclic radicals, indicated hydrogen and thereafter the point of attachment (free valency) have priority for the lowest available number.

Prefixes and Affixes. Prefixes are arranged alphabetically and placed before the parent name; multiplying affixes, if necessary, are inserted and *do not* alter the alphabetical order already attained. The parent name includes any syllables denoting a change of ring member or relating to the structure of a carbon chain. Nondetachable parts of parent names include

- 1. Forming rings: cyclo-, bicyclo-, spiro-;
- 2. Fusing two or more rings: benzo-, naphtho-, imidazo-;
- 3. Substituting one ring or chain member atom for another: oxa-, aza-, thia-;
- 4. Changing positions of ring or chain members: iso-, sec-, tert-, neo-;
- 5. Showing indicated hydrogen;
- 6. Forming bridges: ethano-, epoxy- and;
- 7. Hydro-.

Prefixes that represent complete terminal characteristic groups are preferred to those representing only a portion of a given group. For example, for the group $-C(=O)CH_3$, the prefix (formylmethyl-) is preferred to (oxoethyl-).

The multiplying affixes di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, and so on are used to indicate a set of *identical* unsubstituted radicals or parent compounds. The forms bis-, tris-, tetrakis-, pentakis-, and so on are used to indicate a set of identical radicals or parent compounds *each substituted in the same way*. The affixes bi-, ter-, quater-, quinque-, sexi, septi-, octi-, novi-, deci-, and so on are used to indicate the number of identical rings joined together by a single or double bond.

Although multiplying affixes may be omitted for very common compounds when no ambiguity is caused thereby, such affixes are generally included throughout this handbook in alphabetical listings. An example would be ethyl ether for diethyl ether.

Conjunctive Nomenclature. Conjunctive nomenclature may be applied when a principal group is attached to an acyclic component that is directly attached by a carbon–carbon bond to a cyclic component. The name of the cyclic component is attached directly in front of the name of the acyclic component carrying the principal group. This nomenclature is not used when an unsaturated side chain is named systematically. When necessary, the position of the side chain is indicated by a locant placed before the name of the cyclic component. For substituents on the acyclic chain, carbon atoms of the side chain are indicated by Greek letters proceeding from the principal group to the cyclic component. The terminal carbon atom of acids, aldehydes, and nitriles is omitted when allocating Greek positional letters. Conjunctive nomenclature is not used when the side chain carries more than one of the principal group, except in the case of malonic and succinic acids.

The side chain is considered to extend only from the principal group to the cyclic component. Any other chain members are named as substituents, with appropriate prefixes placed before the name of the cyclic component.

When a cyclic component carries more than one identical side chain, the name of the cyclic component is followed by di-, tri-, etc., and then by the name of the acyclic component, and it is preceded by the locants for the side chains. Examples are

When side chains of two or more different kinds are attached to a cyclic component, only the senior side chain is named by the conjunctive method. The remaining side chains are named as prefixes. Likewise, when there is a choice of cyclic component, the senior is chosen. Benzene derivatives may be named by the conjunctive method only when two or more identical side chains are present. Trivial names for oxo carboxylic acids may be used for the acyclic component. If the cyclic and acyclic components are joined by a double bond, the locants of this bond are placed as superscripts to a Greek capital delta that is

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inserted between the two names. The locant for the cyclic component precedes that for the acyclic component, e.g., indene- $\Delta^{1,\alpha}$ -acetic acid.

Radicofunctional Nomenclature. The procedures of radicofunctional nomenclature are identical with those of substitutive nomenclature except that suffixes are never used. Instead, the functional class name (Table 1.9) of the compound is expressed as one word and the remainder of the molecule as another that precedes the class name. When the functional class name refers to a characteristic group that is bivalent, the two radicals attached to it are each named, and when different, they are written as separate words arranged in alphabetical order. When a compound contains more than one kind of group listed in Table 1.9, that kind is cited as the functional group or class name that occurs higher in the table, all others being expressed as prefixes.

Radicofunctional nomenclature finds some use in naming ethers, sulfides, sulfoxides, sulfones, selenium analogs of the preceding three sulfur compounds, and azides.

TABLE 1.9 Functional Class Names Used in Radicofunctional Nomenclature *Groups are listed in order of decreasing priority*

Group	Functional class names
X in acid derivatives	Name of X (in priority order: fluoride, chloride, bromide, iodide; cyanide, azide; then the sulfur and selenium analogs)
-CN, -NC	Cyanide, isocyanide
>co	Ketone; then S and Se analogs
—ОН	Alcohol; then S and Se analogs
—О—ОН	Hydroperoxide
>0	Ether or oxide
>S, $>$ SO, $>$ SO ₂	Sulfide, sulfoxide, sulfone
>Se, $>$ SeO, $>$ SeO ₂	Selenide, selenoxide, selenone
—F, —Cl, —Br, —I	Fluoride, chloride, bromide, iodide
$-N_3$	Azide

Replacement Nomenclature. Replacement nomenclature is intended for use only when other nomenclature systems are difficult to apply in the naming of chains containing heteroatoms. When no group is present that can be named as a principal group, the longest chain of carbon and heteroatoms terminating with carbon is chosen and named as though the entire chain were that of an acyclic hydrocarbon. The heteroatoms within this chain are identified by means of prefixes aza-, oxa-, thia-, etc., in the order of priority stated in Table 1.3. Locants indicate the positions of the heteroatoms in the chain. Lowest-numbered locants are assigned to the principal group when such is present. Otherwise, lowest-numbered locants are assigned to the heteroatoms considered together and, if there is a choice, to the heteroatoms cited earliest in Table 1.3. An example is

$${\rm HO-\overset{13}{C}H_2-\overset{12}{O}-\overset{11}{C}H_2-\overset{10}{C}H_2-\overset{9}{O}-\overset{8}{C}H_2-\overset{7}{C}H_2-\overset{6}{N}-\overset{5}{C}H_2-\overset{4}{C}H_2-\overset{3}{N}-\overset{2}{C}H_2-\overset{1}{C}OOH}}_{H}$$

13-Hydroxy-9,12-dioxa-3,6-diazatridecanoic acid

Specific Functional Groups

Characteristic groups will now be treated briefly in order to expand the terse outline of substitutive nomenclature presented in Table 1.7. Alternative nomenclature will be indicated whenever desirable.

Acetals and Acytals. Acetals, which contain the group >C(OR)₂, where R may be different, are named (1) as dialkoxy compounds or (2) by the name of the corresponding aldehyde or ketone followed by the name of the hydrocarbon radical(s) followed by the word *acetal*. For example, CH₃—CH(OCH₃)₂ is named either (1) 1,1-dimethoxyethane or (2) acetaldehyde dimethyl acetal.

A cyclic acetal in which the two acetal oxygen atoms form part of a ring may be named (1) as a heterocyclic compound or (2) by use of the prefix methylenedioxy for the group —O—CH₂—O— as a substituent in the remainder of the molecule. For example,

$$\begin{array}{c} O \\ CH_2 \\ \end{array} \tag{1) 1,3-Benzo[d] dioxole-5-carboxylic acid} \\ \\ HOOC \\ O \\ \end{array} \tag{2) 3,4-Methylenedioxybenzoic acid}$$

Acylals, $R^1R^2C(OCOR^3)_2$, are named as acid esters:

$$CH_3-CH_2-CH_2-CH \\ O-CO-CH_2-CH_3 \\ Butylidene acetate propionate$$

 α -Hydroxy ketones, formerly called acyloins, had been named by changing the ending -ic acid or -oic acid of the corresponding acid to -oin. They are preferably named by substitutive nomenclature. For example,

Acid Anhydrides. Symmetrical anhydrides of monocarboxylic acids, when unsubstituted, are named by replacing the word *acid* by *anhydride*. Anhydrides of substituted monocarboxylic acids, if symmetrically substituted, are named by prefixing bis- to the name of the acid and replacing the word *acid* by *anhydride*. Mixed anhydrides are named by giving in alphabetical order the first part of the names of the two acids followed by the word *anhydride*, e.g., acetic propionic anhydride or acetic propanoic anhydride. Cyclic anhydrides of polycarboxylic acids, although possessing a heterocyclic structure, are preferably named as acid anhydrides. For example,

1,8;4,5-Napthalenetetracarboxylic dianhydride. (Note the use of a semicolon to distinguish the pairs of locants.)

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Acyl Halides. Acyl halides, in which the hydroxyl portion of a carboxyl group is replaced by a halogen, are named by placing the name of the corresponding halide after that of the acyl radical. When another group is present that has priority for citation as principal group or when the acyl halide is attached to a side chain, the prefix haloformyl- is used as, for example, in fluoroformyl-.

Alcohols and Phenols. The hydroxyl group is indicated by a suffix -ol when it is the principal group attached to the parent compound and by the prefix hydroxy- when another group with higher priority for citation is present or when the hydroxy group is present in a side chain. When confusion may arise in employing the suffix -ol, the hydroxy group is indicated as a prefix; this terminology is also used when the hydroxyl group is attached to a heterocycle, as, for example, in the name 3-hydroxythiophene to avoid confusion with thiophenol (C_6H_5SH). Designations such as isopropanol, *sec*-butanol, and *tert*-butanol are incorrect because no hydrocarbon exists to which the suffix can be added. Many trivial names are retained. These structures are shown in Table 1.10. The radicals (RO—) are named by adding -oxy as a suffix to the name of the R radical, e.g., pentyloxy for $CH_3CH_2CH_2CH_2CH_2O$ —. These contractions are exceptions: methoxy (CH_3O —), ethoxy (C_2H_5O —), propoxy (C_3H_7O —), butoxy (C_4H_9O —), and phenoxy (C_6H_5O —). For unsubstituted radicals only, one may use isopropoxy [(CH_3)₂CH—O—], isobutoxy [(CH_3)₂CH—O—], *sec*-butoxy [$CH_3CH_2CH(CH_3)$ —O—], and *tert*-butoxy [(CH_3)₂CH—O—].

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures

Ally alcohol	CH ₂ =CHCH ₂ OH
tert-Butyl alcohol	(CH ₃) ₃ COH
Benzyl alcohol	$C_6H_5CH_2OH$
Phenethyl alcohol	C ₆ H ₅ CH ₂ CH ₂ OH
Ethylene glycol	HOCH,CH,OH
1,2-Propylene glycol	CH ₃ CHOHCH ₂ OH
Glycerol	НОСН₂СНОНСН₂ОН
Pentaerythritol	C(CH ₂ OH)₄
Pinacol	$(CH_3)_2COHCOH(CH_3)_2$
Phenol	C ₆ H ₅ OH
	ОН
Xylitol	HOCH₂ÇH−CH−CH₂OH
	OH OH
	On On
Geraniol	$(CH_3)_2C = CHCH_2CH_2C = CHCH_2OH$
	CH ₃
	Cn_3
	CH ₃
Phytol	CH ₂ CH ₂ CHCH ₂ CH ₂ CH(CH ₃) ₂
3	
	CH ₂ CHCH ₂ CH ₂ CH ₂ C=CHCH ₂ OH
	CH ₃ CH ₃
	·

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures (*continued*)

Bivalent radicals of the form O-Y-O are named by adding -dioxy to the name of the bivalent radicals except when forming part of a ring system. Examples are $-O-CH_2-O-(methylenedioxy), -O-CO-O-(carbonyldioxy), and <math>-O-SO_2-O-(sulfonyldioxy)$. Anions derived from alcohols or phenols are named by changing the final -ol to -olate.

zene

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Salts composed of an anion, RO—, and a cation, usually a metal, can be named by citing first the cation and then the RO anion (with its ending changed to -yl oxide), e.g., sodium benzyl oxide for $C_6H_3CH_2ONa$. However, when the radical has an abbreviated name, such as methoxy, the ending -oxy is changed to -oxide. For example, CH_3ONa is named sodium methoxide (not sodium methylate).

Aldehydes. When the group -C(=O)H, usually written -CHO, is attached to carbon at one (or both) end(s) of a linear acyclic chain the name is formed by adding the suffix -al (or -dial) to the name of the hydrocarbon containing the same number of carbon atoms. Examples are butanal for $CH_3CH_2CH_2CHO$ and propanedial for $OHCCH_3CHO$.

Naming an acyclic polyaldehyde can be handled in two ways. (1) When more than two aldehyde groups are attached to an unbranched chain, the proper affix is added to -carbaldehyde, which becomes the suffix to the name of the longest chain carrying the maximum number of aldehyde groups. The name and numbering of the main chain do not include the carbon atoms of the aldehyde groups. (2) The name is formed by adding the prefix formyl- to the name of the -dial that incorporates the principal chain. Any other chains carrying aldehyde groups are named by the use of formylalkyl- prefixes. Examples are

$$\begin{matrix} CHO \\ OHC-CH_2-CH_2-CH_2-CH-CH_2-CHO \end{matrix}$$

- (1) 1,2,5-Pentanetricarbaldehyde
- (2) 3-Formylheptanedial

- (1) 4-(2-Formylethyl)-3-(formylmethyl)-1,2,7-heptanetricarbaldehyde
- (2) 3-Formyl-5-(2-formylethyl)-4-(formylmethyl)nonanedial

When the aldehyde group is directly attached to a carbon atom of a ring system, the suffix -carbaldehyde is added to the name of the ring system, e.g., 2-naphthalenecarbaldehyde. When the aldehyde group is separated from the ring by a chain of carbon atoms, the compound is named (1) as a derivative of the acyclic system or (2) by conjunctive nomenclature, for example, (1) (2-naphthyl)propionaldehyde or (2) 2-naphthalenepropionaldehyde.

An aldehyde group is denoted by the prefix formyl- when it is attached to a nitrogen atom in a ring system or when a group having priority for citation as principal group is present and part of a cyclic system.

When the corresponding monobasic acid has a trivial name, the name of the aldehyde may be formed by changing the ending -ic acid or -oic acid to -aldehyde. Examples are

Formaldehyde Acrylaldehyde (not acrolein)

Acetaldehyde Benzaldehyde Propionaldehyde Cinnamaldehyde

Butyraldehyde 2-Furaldehyde (not furfural)

The same is true for polybasic acids, with the proviso that all the carboxyl groups must be changed to aldehyde; then it is not necessary to introduce affixes. Examples are

Glyceraldehyde Succinaldehyde

Phthalaldehyde (o-, m-, p-) Glycolaldehyde

Malonaldehyde

These trivial names may be retained: citral (3,7-dimethyl-2,6-octadienal), vanillin (4-hydroxy-3-methoxybenzaldehyde), and piperonal (3,4-methylenedioxybenzaldehyde).

Amides. For primary amides the suffix -amide is added to the systematic name of the parent acid. For example, CH₃—CO—NH₂ is acetamide. Oxamide is retained for H₂N— CO—CO—NH₂. The name -carboxylic acid is replaced by -carboxamide.

For amino acids having trivial names ending in -ine, the suffix -amide is added after the name of the acid (with elision of -e for monoamides). For example, H₂N—CH₂—CO— NH₂ is glycinamide.

In naming the radical R—CO—NH—, either (1) the -yl ending of RCO— is changed to -amido or (2) the radicals are named as acylamino radicals. For example,

The latter nomenclature is always used for amino acids with trivial names.

N-substituted primary amides are named either (1) by citing the substituents as N prefixes or (2) by naming the acyl group as an N substituent of the parent compound. For example,

Amines. Amines are preferably named by adding the suffix -amine (and any multiplying affix) to the name of the parent radical. Examples are

> CH₃CH₂CH₂CH₂CH₂NH₂ H₂NCH₂CH₂CH₂CH₂CH₂NH₂
> H₂NCH₂CH₂CH₂CH₂CH₂NH₂

Pentylamine 1,5-Pentyldiamine

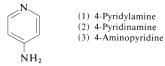
or pentamethylenediamine

Locants of substituents of symmetrically substituted derivatives of symmetrical amines are distinguished by primes or else the names of the complete substituted radicals are enclosed in parentheses. Unsymmetrically substituted derivatives are named similarly or as N-substituted products of a primary amine (after choosing the most senior of the radicals to be the parent amine). For example,

- (1) 1,3'-Diflurodipropylamine
- (2) 1-Fluoro-N-(3-fluoropropyl)propylamine
- (3) (1-Fluoropropyl)(3-fluoropropyl)amine

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Complex cyclic compounds may be named by adding the suffix -amine or the prefix amino- (or aminoalkyl-) to the name of the parent compound. Thus three names are permissible for



Complex linear polyamines are best designated by replacement nomenclature. These trivial names are retained: aniline, benzidene, phenetidine, toluidine, and xylidine.

The bivalent radical —NH— linked to two identical radicals can be denoted by the prefix imino-, as well as when it forms a bridge between two carbon ring atoms. A trivalent nitrogen atom linked to three identical radicals is denoted by the prefix nitrilo-. Thus ethylenedi- aminetetraacetic acid (an allowed exception) should be named ethylenedinitrilotetraacetic acid.

Ammonium Compounds. Salts and hydroxides containing quadricovalent nitrogen are named as a substituted ammonium salt or hydroxide. The names of the substituting radicals precede the word *ammonium*, and then the name of the anion is added as a separate word. For example, $(CH_3)_aN^+I^-$ is tetramethylammonium iodide.

When the compound can be considered as derived from a base whose name does not end in -amine, its quaternary nature is denoted by adding -ium to the name of that base (with elision of -e), substituent groups are cited as prefixes, and the name of the anion is added separately at the end. Examples are

C₆H₅NH₃⁺HSO₄ Anilinium hydrogen sulfate [(C₆H₅NH₃)⁺PtCl₆⁻ Dianilinium hexachloroplatinate

The names *choline* and *betaine* are retained for unsubstituted compounds.

In complex cases, the prefixes amino- and imino- may be changed to ammonio- and iminio- and are followed by the name of the molecule representing the most complex group attached to this nitrogen atom and are preceded by the names of the other radicals attached to this nitrogen. Finally the name of the anion is added separately. For example, the name might be 1-trimethylammonioacridine chloride or 1-acridinyltrimethylammonium chloride.

When the preceding rules lead to inconvenient names, then (1) the unaltered name of the base may be used followed by the name of the anion or (2) for salts of hydrohalogen acids only the unaltered name of the base is used followed by the name of the hydrohalide. An example of the latter would be 2-ethyl-p-phenylenediamine monohydrochloride.

Azo Compounds. When the azo group (-N = N -) connects radicals derived from identical unsubstituted molecules, the name is formed by adding the prefix azo- to the name of the parent unsubstituted molecules. Substituents are denoted by prefixes and suffixes. The azo group has priority for lowest-numbered locant. Examples are azobenzene for $C_6H_5-N=N-C_6H_5$, azobenzene-4- sulfonic acid for $C_6H_5-N=N-C_6H_5SO_3H$, and 2',4-dichloroazobenzene-4'-sulfonic acid for $ClC_6H_4-N=N-C_6H_3ClSO_3H$.

When the parent molecules connected by the azo group are different, azo is placed between the complete names of the parent molecules, substituted or unsubstituted. Locants are placed between the affix azo and the names of the molecules to which each refers. Preference is given to the more complex parent molecule for citation as the first component, e.g., 2-aminonaphthalene-1-azo-(4'-chloro-2'-methylbenzene).

In an alternative method, the senior component is regarded as substituted by RN=N—, this group R being named as a radical. Thus 2-(7-phenylazo-2-naphthylazo)anthracene is the name by this alternative method for the compound named anthracene-2-azo-2'-naphthalene-7'-azobenzene.

Azoxy Compounds. Where the position of the azoxy oxygen atom is unknown or immaterial, the compound is named in accordance with azo rules, with the affix azo replaced by azoxy. When the position of the azoxy oxygen atom in an unsymmetrical compound is designated, a prefix NNO- or ONN- is used. When both the groups attached to the azoxy radical are cited in the name of the compound, the prefix NNO- specifies that the second of these two groups is attached directly to -N(O)—; the prefix ONN- specifies that the first of these two groups is attached directly to -N(O)—. When only one parent compound is cited in the name, the prefixed ONN- and NNO- specify that the group carrying the primed and unprimed substituents is connected, respectively, to the -N(O)— group. The prefix NON- signifies that the position of the oxygen atom is unknown; the azoxy group is then written as $-N_2O$ —. For example,

2,2',4-Trichloro-NNO-azoxybenzene

Boron Compounds. Molecular hydrides of boron are called boranes. They are named by using a multiplying affix to designate the number of boron atoms and adding an Arabic numeral within parentheses as a suffix to denote the number of hydrogen atoms present. Examples are pentaborane(9) for B_5H_9 and pentaborane(11) for B_5H_{11} .

Organic ring systems are named by replacement nomenclature. Three- to ten-membered monocyclic ring systems containing uncharged boron atoms may be named by the specialist nomenclature for heterocyclic systems. Organic derivatives are named as outlined for substitutive nomenclature. The complexity of boron nomenclature precludes additional details; the text by Rigaudy and Klesney should be consulted.

Carboxylic Acids. Carboxylic acids may be named in several ways. (1) —COOH groups replacing CH₃— at the end of the main chain of an acyclic hydrocarbon are denoted by adding -oic acid to the name of the hydrocarbon. (2) When the —COOH group is the principal group, the suffix -carboxylic acid can be added to the name of the parent chain whose name and chain numbering *does not include* the carbon atom of the —COOH group. The former nomenclature is preferred unless use of the ending -carboxylic acid leads to citation of a larger number of carboxyl groups as suffix. (3) Carboxyl groups are designated by the prefix carboxy- when attached to a group named as a substituent or when another group is present that has higher priority for citation as principal group. In all cases, the

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principal chain should be linked to as many carboxyl groups as possible even though it might not be the longest chain present. Examples are

Removal of the OH from the —COOH group to form the acyl radical results in changing the ending -oic acid to -oyl or the ending -carboxylic acid to -carbonyl. Thus the radical CH₃CH₂CH₂CH₂CO— is named either pentanoyl or butanecarbonyl. When the hydroxyl has not been removed from all carboxyl groups present in an acid, the remaining carboxyl groups are denoted by the prefix carboxy-. For example, HOOCCH₂CH₂CH₂CH₂CH₂CO— is named 6-carboxyhexanoyl.

Many trivial names exist for acids: these are listed in Table 1.11. Generally, radicals are formed by replacing -ic acid by -oyl.* When a trivial name is given to an acyclic monoacid or diacid, the numeral 1 is always given as locant to the carbon atom of a carboxyl group in the acid or to the carbon atom with a free valence in the radical RCO—.

Ethers $(R^1 - O - R^2)$. In substitutive nomenclature, one of the possible radicals, R—O—, is stated as the prefix to the parent compound that is senior from among R¹ or R². Examples are methoxyethane for CH₃OCH₂CH₃ and butoxyethanol for C₄H₉OCH₂CH₂OH.

When another principal group has precedence and oxygen is linking two identical parent compounds, the prefix oxy- may be used, as with 2,2'-oxydiethanol for HOCH₂CH₂OCH₂CH₂OH.

Compounds of the type RO—Y—OR, where the two parent compounds are identical and contain a group having priority over ethers for citation as suffix, are named as assemblies of identical units. For example, HOOC—CH₂—O—CH₂CH₂—O—CH₂—COOH is named 2,2'-(ethylenedioxy)diacetic acid.

Linear polyethers derived from three or more molecules of aliphatic dihydroxy compounds, particularly when the chain length exceeds ten units, are most conveniently named by open-chain replacement nomenclature. For example, $CH_3CH_2-O-CH_2CH_2-O-CH_2CH_3$ could be 3,6-dioxaoctane or (2-ethoxy)ethoxyethane.

Symmetrical linear polyethers may be named (1) in terms of the central oxygen atom when there is an odd number of ether oxygen atoms or (2) in terms of the central hydrocarbon group when there is an even number of ether oxygen atoms. For example, $C_2H_5 - O - C_4H_8 - O - C_2H_5$ is bis-(4-ethoxybutyl)ether, and 3,6-dioxaoctane (earlier example) could be named 1,2-bis(ethoxy)ethane.

Polyethers and Cyclic Polyethers. During the past several decades, linear and cyclic polyethers have gained considerable prominence. This is largely due to their remarkable ability to complex metallic and organic cations. The linear polyethers of the polyethylene

^{*}Exceptions: formyl, acetyl, propionyl, butyryl, isobutyryl, valeryl, isovaleryl, oxalyl, malonyl, succinyl, glutaryl, furoyl, and thenoyl.

TABLE 1.11 Names of Some Carboxylic Acids

Systematic name	Trivial name	Systematic name	Trivial name
Methanoic	Formic	trans-Methylbutenedioic	Mesaconic*
Ethanoic	Acetic		111000001110
Propanoic	Propionic	1,2,2-Trimethyl-1,3-	Camphoric
Butanoic	Butyric	cyclopentanedicarboxylic	cumpnone
2-Methylpropanoic	Isobutyric*	acid	
Pentanoic	Valeric	Benzenecarboxylic	Benzoic
3-Methylbutanoic	Isovaleric*	1,2-Benzenedicarboxylic	Phthalic
2,2-Dimethylpropanoic	Pivalic*	1,3-Benzenedicarboxylic	Isophthalic
Hexanoic	(Caproic)	1,4-Benzenedicarboxylic	Terephthalic
Heptanoic	(Enanthic)	Naphthalenecarboxylic	Naphthoic
Octanoic	(Caprylic)	Methylbenzenecarboxylic	Toluic
Decanoic	(Capric)	2-Phenylpropanoic	Hydratropic
Dodecanoic	Lauric*	2-Phenylpropenoic	Atropic
Tetradecanoic	Myristic*	trans-3-Phenylpropenoic	Cinnamic
Hexadecanoic	Palmitic*	Furancarboxylic	Furoic
Octadecanoic Stearic*		Thiophenecarboxylic	Thenoic
		3-Pyridinecarboxylic	Nicotinic
Ethanedioic	Oxalic	4-Pyridinecarboxylic	Isonicotinic
Propanedioic	Malonic		
Butanedioic	Succinic	Hydroxyethanoic	Glycolic
Pentanedioic	Glutaric	2-Hydroxypropanoic	Lactic
Hexanedioic	Adipic	2,3-Dihydroxypropanoic	Glyceric
Heptanedioic	Pimelic*	Hydroxypropanedioic	Tartronic
Octanedioic	Suberic*	Hydroxybutanedioic	Malic
Nonanedioic	Azelaic*	2,3-Dihydroxybutanedioic	Tartaric
Decanedioic	Sebacic*	3-Hydroxy-2-phenylpropanoic	Tropic
Propenoic	Acrylic	2-Hydroxy-2,2-	Benzilic
Propynoic	Propiolic	diphenylethanoic	
2-Methylpropenoic	Methacrylic	2-Hydroxybenzoic	Salicylic
trans-2-Butenoic	Crotonic	Methoxybenzoic	Anisic
cis-2-Butenoic	Isocrotonic	4-Hydroxy-3-methoxybenzoic	Vanillic
cis-9-Octadecenoic	Oleic		
trans-9-Octadecenoic	Elaidic	3,4-Dimethoxybenzoic	Veratric
cis-Butenedioic	Maleic	3,4-Methylenedioxybenzoic	Piperonylic
trans-Butenedioic	Fumaric	3,4-Dihydroxybenzoic	Protocatechui
cis-Methylbutenedioic	Citraconic*	3,4,5-Trihydroxybenzoic	Gallic

The names in parentheses are abandoned but are listed for reference to older literature.

glycol type are discussed in Section 10. The cyclic polyethers are called crown ethers if they are monocyclic and cryptands if they are di- or multi-cyclic compounds.

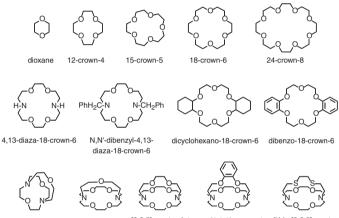
Crown ethers are typically complicated structures and their names have evolved from the convenient, semi-systematic nomenclature developed by the pioneers in the field. The name "crown" was suggested because the cyclic polyethers "crown a cation" when they complex it. The most general naming system consists in identifying the largest cycle and then denoting the number and type of heteroatoms present. The most common repeating unit is ethyleneoxy or —CH₂CH₂O—, normally in the form 1,2-ethylenedioxy and this is

^{*} Systematic names should be used in derivatives formed by substitution on a carbon atom.

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presumed to be present unless otherwise noted. Ethylene oxide (oxirane) is the smallest cyclic compound containing this unit. Dioxane is formally its dimer. The trimer, called 9-crown-3, is known but the smallest compound normally considered to be a crown ether is 12-crown-4. 18-Crown-6 has six repeating ethyleneoxy units and is systematically named 1,4,7,10.13,16-hexaoxacyclooctadecane.

Examples of various crown ethers and cryptands are shown here. The top line of compounds may be named readily enough although the problem with this semi-systematic approach is obvious. If two methylenes were added to 18-crown-6, the compound could correctly be called 20-crown-6 but in the absence of unequivocal descriptors, the positions of the 3-carbon bridges would be unclear. The more cumbersome name 1,4,7,11,13,17-hexaoxacy-cloicosane tells clearly that the longer bridges are adjacent to each other. A similar problem is apparent in the last two entries of the second line. The designations dicyclohexano and dibenzo are clear as to the substituents but not their positions. The semi-systematic nomenclature is widely used, however, because it is so much less cumbersome for most purposes.



[1.1.1] cryptand [2.2.1] cryptand [2.2.2] cryptand benzo-[2.2.2] cryptand dithia-[2.2.2] cryptand

An additional nuance in the nomenclature of these compounds concerns their complexes. The open-chained compounds are often referred to as podands and their complexes as podates. The cyclic ethers may also be called coronands and their complexes are therefore coronates. Complexed cryptands are cryptates. The even more complicated structures known as spherands, cavitands, or carcerands are called spherates, cavitates, or carcerates, respectively, when complexed. The combination of a macrocycle (crown ether or coronand) and a sidechain (podand) is typically called a lariat ether.

An alternate nomenclature system based upon IUPAC principles polymer systems has also been developed but it has not been adopted broadly. Using this method, 15-crown-5 would be called cyclo[pentakis(oxyethylene)] instead of 1,4,7,10,13-pentaoxacyclopentadecane. In this case, substituents and other heteroatoms make the names more complex.

Partial ethers of polyhydroxy compounds may be named (1) by substitutive nomenclature or (2) by stating the name of the polyhydroxy compound followed by the name of the etherifying radical(s) followed by the word *ether*. For example,

Cyclic ethers are named either as heterocyclic compounds or by specialist rules of heterocyclic nomenclature. Radicofunctional names are formed by citing the names of the radicals R¹ and R² followed by the word *ether*. Thus methoxyethane becomes ethyl methyl ether and ethoxyethane becomes diethyl ether.

Halogen Derivatives. Using substitutive nomenclature, names are formed by adding prefixes listed in Table 1.8 to the name of the parent compound. The prefix perhalo- implies the replacement of all hydrogen atoms by the particular halogen atoms.

Cations of the type $R^1R^2X^+$ are given names derived from the halonium ion, H_2X^+ , by substitution, e.g., diethyliodonium chloride for $(C_2H_5)_2I^+CI^-$.

These trivial names are retained: bromoform (CHBr₃), chloroform (CHCl₃), fluoroform (CHF₃), iodoform (CHI₃), phosgene (COCl₂), thiophosgene (CSCl₂), and dichlorocarbene radical (\geq CCl₂). Inorganic nomenclature leads to such names as carbonyl and thiocarbonyl halides (COX₂ and CSX₂) and carbon tetrahalides (CX₄).

Hydroxylamines and Oximes. For RNH—OH compounds, prefix the name of the radical R to hydroxylamine. If another substituent has priority as principal group, attach the prefix hydroxylamino- to the parent name. For example, C_6H_5 NHOH would be named *N*-phenylhydroxylamine, but HOC_6H_4 NHOH would be (hydroxylamino)phenol, with the point of attachment indicated by a locant preceding the parentheses.

Compounds of the type $R^1NH - OR_2$ are named (1) as alkoxyamino derivatives of compound R^1H , (2) as N,O-substituted hydroxylamines, (3) as alkoxyamines (even if R^1 is hydrogen), or (4) by the prefix aminooxy- when another substituent has priority for parent name. Examples of each type are as follows:

- 1. 2-(Methoxyamino)-8-naphthalenecarboxylic acid for CH₃ONH—C₁₀H₆COOH
- 2. *O*-phenylhydroxylamine for $H_2N-O-C_6H_5$ or *N*-phenylhydroxylamine for C_6H_5NH-OH
- 3. Phenoxyamine for $H_2N O C_6H_5$ (not preferred to *O*-phenylhydroxylamine)
- 4. Ethyl (aminooxy)acetate for H₂N-O-CH₂CO-OC₂H₅

Acyl derivatives, RCO—NH—OH and H_2N —O—CO—R, are named as *N*-hydroxy derivatives of amides and as *O*-acylhydroxylamines, respectively. The former may also be named as hydroxamic acids. Examples are *N*-hydroxyacetamide for CH_3CO —NH—OH and *O*-acetylhydroxylamine for H_2N —O—CO— CH_3 . Further substituents are denoted by prefixes with *O*- and/or *N*-locants. For example, C_6H_5NH —O— C_2H_5 would be *O*-ethyl-*N*-phenylhydroxylamine or *N*-ethoxylaniline.

For oximes, the word *oxime* is placed after the name of the aldehyde or ketone. If the carbonyl group is not the principal group, use the prefix hydroxyimino-. Compounds with the group >N—OR are named by a prefix alkyloxyimino- as oxime *O*-ethers or as *O*-substituted oximes. Compounds with the group >C = N(O)R are named by adding *N*-oxide after the name of the alkylideneamine compound. For amine oxides, add the word *oxide* after the name of the base, with locants. For example, C_3H_3N —O is named pyridine *N*-oxide or pyridine 1-oxide.

Imines. The group > C = NH is named either by the suffix -imine or by citing the name of the bivalent radical $R^1R^2C \le as$ a prefix to amine. For example, $CH_3CH_2CH = NH$

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could be named 1-butanimine or butylideneamine. When the nitrogen is substituted, as in $CH_2=N-CH_3$, the name is N-(methylidene) ethylamine.

Quinones are exceptions. When one or more atoms of quinonoid oxygen have been replaced by >NH or >NR, they are named by using the name of the quinone followed by the word *imine* (and preceded by proper affixes). Substituents on the nitrogen atom are named as prefixes. Examples are

$$O \longrightarrow NH$$
 p -Benzoquinone monoimine P -Benzoquinone diimine

Ketenes. Derivatives of the compound ketene, $CH_2=C=O$, are named by substitutive nomenclature. For example, $C_4H_9CH=C=O$ is butyl ketene. An acyl derivative, such as $CH_3CH_2-CO-CH_2CH=C=O$, may be named as a polyketone, 1-hexene-1,4-dione. Bis-ketene is used for two to avoid ambiguity with diketene (dimeric ketene).

Ketones. Acyclic ketones are named (1) by adding the suffix -one to the name of the hydrocarbon forming the principal chain or (2) by citing the names of the radicals R^1 and R^2 followed by the word *ketone*. In addition to the preceding nomenclature, acyclic monoacyl derivatives of cyclic compounds may be named (3) by prefixing the name of the acyl group to the name of the cyclic compound. For example,

When the cyclic component is benzene or naphthalene, the -ic acid or -oic acid of the acid corresponding to the acyl group is changed to -ophenone or -onaphthone, respectively. For example, $C_6H_5-CO-CH_2CH_2CH_3$ can be named either butyrophenone (or butanophenone) or phenyl propyl ketone.

Radicofunctional nomenclature can be used when a carbonyl group is attached directly to carbon atoms in two ring systems and no other substituent is present having priority for citation.

When the methylene group in polycarbocyclic and heterocyclic ketones is replaced by a keto group, the change may be denoted by attaching the suffix -one to the name of the ring system. However, when \ge CH in an unsaturated or aromatic system is replaced by a keto group, two alternative names become possible. (1) The maximum number of noncumulative double bonds is added after introduction of the carbonyl group(s), and any hydrogen that remains to be added is denoted as indicated hydrogen with the carbonyl group having priority over the indicated hydrogen for lower-numbered locant. (2) The prefix oxois used, with the hydrogenation indicated by hydro prefixes; hydrogenation is considered

to have occurred before the introduction of the carbonyl group. For example,

$$\begin{array}{c|c} \mathbf{O} \\ || \\ \mathbf{C} \\ \mathbf{CH_2} \\ (1) \ 1(2H) \text{-Naphthalenone} \\ (2) \ 1\text{-Oxo-1,2-dihydronaphthalene} \end{array}$$

When another group having higher priority for citation as principal group is also present, the ketonic oxygen may be expressed by the prefix oxo-, or one can use the name of the carbonyl-containing radical, as, for example, acyl radicals and oxo-substituted radicals. Examples are

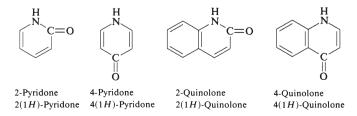
HOOC
$$\stackrel{2}{\stackrel{3}{\stackrel{}}}$$
 $\stackrel{1}{\stackrel{}}$ $\stackrel{1}{\stackrel{}}$ $\stackrel{2}{\stackrel{}}$ $\stackrel{3}{\stackrel{}}$ $\stackrel{1}{\stackrel{}}$ $\stackrel{5}{\stackrel{}}$ $\stackrel{6}{\stackrel{}}$ $\stackrel{6}{\stackrel{}}$ $\stackrel{4}{\stackrel{}}$ $\stackrel{4}{\stackrel{4}}$ $\stackrel{4}}$ $\stackrel{4}$ $\stackrel{4}{\stackrel{4}}$ $\stackrel{4}$ $\stackrel{4}}$ $\stackrel{4}$ $\stackrel{4}$ $\stackrel{4}$ $\stackrel{4}$ $\stackrel{4}$ $\stackrel{4$

Diketones and tetraketones derived from aromatic compounds by conversion of two or four \geq CH groups into keto groups, with any necessary rearrangement of double bonds to a quinonoid structure, are named by adding the suffix -quinone and any necessary affixes.

Polyketones in which two or more contiguous carbonyl groups have rings attached at each end may be named (1) by the radicofunctional method or (2) by substitutive nomenclature. For example,

Some trivial names are retained: acetone (2-propanone), biacetyl (2,3-butanedione), propiophenone (C_6H_5 —CO— CH_2CH_3), chalcone (C_6H_5 —CH=CH—CO— C_6H_5), and deoxybenzoin (C_6H_5 — CH_2 —CO— C_6H_5).

These contracted names of heterocyclic nitrogen compounds are retained as alternatives for systematic names, sometimes with indicated hydrogen. In addition, names of oxo derivatives of fully saturated nitrogen heterocycles that systematically end in -idinone are often contracted to end in -idone when no ambiguity might result. For example,



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Lactones, Lactides, Lactams, and Lactims. When the hydroxy acid from which water may be considered to have been eliminated has a trivial name, the lactone is designated by substituting -olactone for -ic acid. Locants for a carbonyl group are numbered as low as possible, even before that of a hydroxyl group.

Lactones formed from aliphatic acids are named by adding -olide to the name of the nonhydroxylated hydrocarbon with the same number of carbon atoms. The suffix -olide signifies the change of >CH \cdots CH $_3$ into >C \cdots C=O

Structures in which one or more (but not all) rings of an aggregate are lactone rings are named by placing -carbolactone (denoting the —O—CO—bridge) after the names of the structures that remain when each bridge is replaced by two hydrogen atoms. The locant for —CO— is cited before that for the ester oxygen atom. An additional carbon atom is incorporated into this structure as compared to the -olide.

These trivial names are permitted: γ -butyrolactone, γ -valerolactone, and δ -valerolactone. Names based on heterocycles may be used for all lactones. Thus, γ -butyrolactone is also tetrahydro-2-furanone or dihydro-2(3H)-furanone.

Lactides, intermolecular cyclic esters, are named as heterocycles. *Lactams* and *lactims*, containing a -CO-NH- and -C(OH)=N- group, respectively, are named as heterocycles, but they may also be named with -lactam or -lactim in place of -olide. For example,

Nitriles and Related Compounds. For acids whose systematic names end in -carboxylic acid, nitriles are named by adding the suffix -carbonitrile when the —CN group replaces the —COOH group. The carbon atom of the —CN group is excluded from the numbering of a chain to which it is attached. However, when the triple-bonded nitrogen atom is considered to replace three hydrogen atoms at the end of the main chain of an acyclic hydrocarbon, the suffix -nitrile is added to the name of the hydrocarbon. Numbering begins with the carbon attached to the nitrogen. For example, CH₃CH₂CH₂CH₂CH₂CN is named (1) pentanecarbonitrile or (2) hexanenitrile.

Trivial acid names are formed by changing the endings -oic acid or -ic acid to -onitrile. For example, CH₃CN is acetonitrile. When the —CN group is not the highest priority group, the —CN group is denoted by the prefix cyano-.

In order of decreasing priority for citation of a functional class name, and the prefix for substitutive nomenclature, are the following related compounds:

Functional group	Prefix	Radicofunctional ending	
—NC	Isocyano-	Isocyanide	
—OCN	Cyanato-	Cyanate	
—NCO	Isocyanato-	Isocyanate	
—ONC	_ `	Fulminate	
—SCN	Thiocyanato-	Thiocyanate	
—NCS	Isothiocyanato-	Isothiocyanate	
—SeCN	Selenocyanato-	Selenocyanate	
—NCSe	Isoselenocyanato-	Isoselenocyanate	

Peroxides. Compounds of the type R-O-OH are named (1) by placing the name of the radical R before the word *hydroperoxide* or (2) by use of the prefix hydroperoxy-when another parent name has higher priority. For example, C_2H_5OOH is ethyl hydroperoxide.

Compounds of the type $R^1O - OR^2$ are named (1) by placing the names of the radicals in alphabetical order before the word *peroxide* when the group -O - O - links two chains, two rings, or a ring and a chain, (2) by use of the affix dioxy to denote the bivalent group -O - O - for naming assemblies of identical units or to form part of a prefix, or (3) by use of the prefix epidioxy- when the peroxide group forms a bridge between two carbon atoms, a ring, or a ring system. Examples are methyl propyl peroxide for $CH_3 - O - C - C_3H_7$ and 2,2'- dioxydiacetic acid for $HOOC - CH_2 - O - C - CH_2 - COOH$.

Phosphorus Compounds. Acyclic phosphorus compounds containing only one phosphorus atom, as well as compounds in which only a single phosphorus atom is in each of several functional groups, are named as derivatives of the parent structures listed in Table 1.12. Often these are purely hypothetical parent structures. When hydrogen attached to phosphorus is replaced by a hydrocarbon group, the derivative is named by substitution nomenclature. When hydrogen of an —OH group is replaced, the derivative is named by radicofunctional nomenclature. For example, $C_2H_5PH_2$ is ethylphosphine; $(C_2H_5)_2PH$, diethylphosphine; $(C_3H_5)_2PH$, diethylpho

Salts and Esters of Acids. Neutral salts of acids are named by citing the cation(s) and then the anion, whose ending is changed from -oic to -oate or from -ic to -ate. When different acidic residues are present in one structure, prefixes are formed by changing the anion ending -ate to -ato- or -ide to -ido-. The prefix carboxylato- denotes the ionic group —COO⁻. The phrase: (metal) salt of (the acid) is permissible when the carboxyl groups are not all named as affixes.

Acid salts include the word *hydrogen* (with affixes, if appropriate) inserted between the name of the cation and the name of the anion (or word *salt*).

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TABLE 1.12	Parent Structures of Phosphorus-containing Compounds
IADLL 1.12	i archi su uctures of i nosphorus-containing compound

Formula	Parent name	Substitutive prefix	Radicofunctional ending
H ₃ P H ₅ P	Phosphine Phosphorane	H ₂ P — Phosphino- H ₄ P — Phosphoranyl- H ₃ P < Phosphoroanediyl- H ₂ P ≤ Phosphoranetriyl-	Phosphide — — —
H ₃ PO H ₃ PS H ₃ PNH P(OH) ₃ HP(OH) ₂ H ₂ POH P(O)(OH) ₃ HP(O)(OH) ₂ H ₂ P(O)OH	Phosphine oxide Phosphine sulfide Phosphine imide Phosphorous acid Phosphonous acid Phosphinous acid Phosphoric acid Phosphonic acid Phosphonic acid	—————————————————————————————————————	Phosphite Phosphonite Phosphinite Phosphate(V) Phosphonate — Phosphinate

Esters are named similarly, with the name of the alkyl or aryl radical replacing the name of the cation. Acid esters of acids and their salts are named as neutral esters, but the components are cited in the order: cation, alkyl or aryl radical, hydrogen, and anion. Locants are added if necessary. For example,

$$\begin{array}{cccc} CH_2-CO-OC_2H_5 \\ HOC-COO^- \\ CH_2-COO^- \\ CH_2-COO^- \end{array} \\ \begin{array}{ccccc} Potassium \ 1\text{-ethyl hydrogen citrate} \\ Potassium \ 2\text{-ethyl hydrogen citrat$$

Ester groups in R¹—CO—OR² compounds are named (1) by the prefix alkoxycarbonylor aryloxycabonyl- for —CO—OR² when the radical R¹ contains a substituent with priority for citation as principal group or (2) by the prefix acyloxy- for R¹—CO—O— when the radical R² contains a substituent with priority for citation as principal group. Examples are

$$CH_2CH_2CO-OCH_3 \\ CO-OCH_3 \\ [CH_3O-CO-CH_2CH_2\dot{N}(CH_3)_3] Cl^- \\ [(2-Methoxycarbonyl)ethyl]trimethylammonium chloride \\ C_6H_5-CO-OCH_2CH_2COOH \\ 3-Benzoyloxypropionic acid$$

The trivial name *acetoxy* is retained for the CH_3 —CO—O— group. Compounds of the type $R^2C(OR^2)_3$ are named as R^2 esters of the hypothetical ortho acids. For example, $CH_3C(OCH_3)_3$ is trimethyl orthoacetate.

Silicon Compounds. SiH₄ is called silane; its acyclic homologs are called disilane, trisilane, and so on, according to the number of silicon atoms present. The chain is numbered from one end to the other so as to give the lowest-numbered locant in radicals to the free valence or to substituents on a chain. The abbreviated form silyl is used for the radical SiH_3 —. Numbering and citation of side chains proceed according to the principles set forth for hydrocarbon chains. Cyclic nonaromatic structures are designated by the prefix cyclo-.

When a chain or ring system is composed entirely of alternating silicon and oxygen atoms, the parent name *siloxane* is used with a multiplying affix to denote the number of silicon atoms present. The parent name *silozane* implies alternating silicon and nitrogen atoms; multiplying affixes denote the number of silicon atoms present.

The prefix sila- designates replacement of carbon by silicon in replacement nomenclature. Prefix names for radicals are formed analogously to those for the corresponding carbon-containing compounds. Thus silyl is used for SiH₃—, silyene for —SiH₂—, silylidyne for —SiH<.

Sulfur Compounds

Bivalent Sulfur. The prefix thio-, placed before an affix that denotes the oxygen-containing group or an oxygen atom, implies the replacement of that oxygen by sulfur. Thus the suffix -thiol denotes —SH, -thione denotes —(C)=S and implies the presence of an =S at a nonterminal carbon atom, -thioic acid denotes $[(C)=S]OH \rightleftharpoons [(C)=O]SH$ (that is, the O-substituted acid and the S-substituted acid, respectively), -dithioic acid denotes [-C(S)]SH, and -thial denotes —(C)HS (or -carbothialdehyde denotes —CHS). When -carboxylic acid has been used for acids, the sulfur analog is named -carbothioic acid or -carbodithioic acid.

Prefixes for the groups HS— and RS— are mercapto- and alkylthio-, respectively; this latter name may require parentheses for distinction from the use of thio- for replacement of oxygen in a trivially named acid. Examples of this problem are $4\text{-}C_2H_5$ — C_6H_4 —CSOH named p-ethyl(thio)benzoic acid and $4\text{-}C_2H_5$ —S— C_6H_4 —COOH named p-(ethylthio) benzoic acid. When —SH is not the principal group, the prefix mercapto- is placed before the name of the parent compound to denote an unsubstituted —SH group.

The prefix thioxo- is used for naming = S in a thioketone. Sulfur analogs of acetals are named as alkylthio- or arylthio-. For example, $CH_3CH(SCH_3)OCH_3$ is 1-methoxy-1-(methylthio)ethane. Prefix forms for -carbothioic acids are hydroxy(thiocarbonyl)- when referring to the *O*-substituted acid and mercapto(carbonyl)- for the *S*-substituted acid.

Salts are formed as with oxygen-containing compounds. For example, C_2H_5 —S—Na is named either sodium ethanethiolate or sodium ethyl sulfide. If mercapto- has been used as a prefix, the salt is named by use of the prefix sulfido- for —S⁻.

Compounds of the type $R^1 - S - R^2$ are named alkylthio- (or arylthio-) as a prefix to the name of R^1 or R^2 , whichever is the senior.

Sulfonium Compounds. Sulfonium compounds of the type $R^1R^2R^3S^+X^-$ are named by citing in alphabetical order the radical names followed by -sulfonium and the name of the anion. For heterocyclic compounds, -ium is added to the name of the ring system. Replacement of >CH by sulfonium sulfur is denoted by the prefix thionia-, and the name of the anion is added at the end.

Organosulfur Halides. When sulfur is directly linked only to an organic radical and to a halogen atom, the radical name is attached to the word *sulfur* and the name(s) and number of the halide(s) are stated as a separate word. Alternatively, the name can be formed from R—SOH, a sulfenic acid whose radical prefix is sulfenyl-. For example, CH₃CH₂—S—Br would be named either ethylsulfur monobromide or ethanesulfenyl bromide. When another principal group is present, a composite prefix is formed from the number and substitutive name(s) of the halogen atoms in front of the syllable thio. For example, BrS—COOH is (bromothio)formic acid.

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Sulfoxides. Sulfoxides, R¹—SO—R², are named by placing the names of the radicals in alphabetical order before the word *sulfoxide*. Alternatively, the less senior radical is named followed by sulfinyl- and concluded by the name of the senior group. For example, CH₃CH₂—SO—CH₂CH₂CH₃ is named either ethyl propyl sulfoxide or 1-(ethylsulfinyl)-propane.

When an >SO group is incorporated in a ring, the compound is named an oxide.

Sulfones. Sulfones, $R^1 - SO_2 - R^2$, are named in an analogous manner to sulfoxides, using the word *sulfone* in place of *sulfoxide*. In prefixes, the less senior radical is followed by -sulfonyl-. When the $> SO_2$ group is incorporated in a ring, the compound is named as a dioxide.

Sulfur Acids. Organic oxy acids of sulfur, that is, —SO₃H, —SO₂H, and —SOH, are named sulfonic acid, sulfinic acid, and sulfenic acid, respectively. In subordinate use, the respective prefixes are sulfo-, sulfino, and sulfeno-. The grouping —SO₂—O—SO₂— or —SO—O—SO is named sulfonic or sulfinic anhydride, respectively.

Inorganic nomenclature is employed in naming sulfur acids and their derivatives in which sulfur is linked only through oxygen to the organic radical. For example, $(C_2H_5O)_2SO_2$ is diethyl sulfate and $C_2H_5O-SO_2$ —OH is ethyl hydrogen sulfate. Prefixes O- and S- are used where necessary to denote attachment to oxygen and to sulfur, respectively, in sulfur replacement compounds. For example, CH_3 —S— SO_2 —ONa is sodium S-methyl thiosulfate.

When sulfur is linked only through nitrogen, or through nitrogen and oxygen, to the organic radical, naming is as follows: (1) N-substituted amides are designated as N-substituted derivatives of the sulfur amides and (2) compounds of the type $R-NH-SO_3H$ may be named as N-substituted sulfamic acids or by the prefix sulfoamino- to denote the group HO_3S-NH- . The groups -N=SO and $-N=SO_2$ are named sulfinylamines and sulfonylamines, respectively.

Sultones and Sultams. Compounds containing the group $-SO_2-O-$ as part of the ring are called -sultone. The $-SO_2-$ group has priority over the -O- group for lowest-numbered locant.

Similarly, the $-SO_2-N=$ group as part of a ring is named by adding -sultam to the name of the hydrocarbon with the same number of carbon atoms. The $-SO_2-$ has priority over -N= for lowest-numbered locant.

Steroids. Steroids are important natural products that have a special nomenclature. They typically consist of three fused 6-membered rings and a four fused 5-membered ring. The

rings are designated A, B, C, and D as shown here. The most common, all *trans* ring fusion is illustrated in the right hand structure. Most steroids that occur naturally possess the two methyl groups ("bridgehead" or angular methyl groups) shown as carbons 18 and 19 at positions 10 and 13, respectively.

Cholesterol is the most common steroid of mammalian membranes. It is formed biologically from lanosterol, as shown. Ergosterol is the most common steroid of fungal membranes. It differs from cholesterol by the presence of two additional double bonds that affect its three dimensional structure. Also shown are three so-called steroid hormones, androsterone, estradiol, and testosterone. Note the presence of an aromatic A-ring in estradiol.

Vitamins. The vitamins are natural organic compounds of considerable diversity that occur widely. The name derives from the Latin *vita* (life) and "amin," a shortened form of amine. The name reflects the historical discovery of these substances, not all of which are amines. They are all of relatively low molecular weight, especially compared to peptides but in a range comparable to steroids. These substances are uniformly active and play various roles in biosynthesis and metabolism. The vitamins are too numerous to detail here but the most common examples are illustrated. They are classed using the common system, that is, water or fat soluble, depending on their approximate level of hydrophobicity or hydrophilicity. Their names are typically nonsystematic but the diversity of their structures requires that the trivial names be used.

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Biological Nomenclature

The names assigned to compounds by organic chemists and biologists sometimes differ. Moreover, biological structures are made up of repeating components and rapidly become large and complex molecules. Thus, special terminology has been developed to assist in describing these compounds.

Amino Acids. An amino acid is any organic compound that possesses both amine $(-NH_2)$ and carboxyl (-COOH) groups within the same organic framework. When both functional groups are attached to the same carbon atom, they are designated α -amino acids. These are of special significance in biology as they form the diverse monomer set from which peptides and proteins are built.

Aminoacetic acid is the simplest example of an α -amino acid. Among the 20 biologically most important amino acids, its structure is unique in two ways. First, it possesses no "sidechain" attached to the methylene carbon. Second, the lack of any substituent (other than hydrogen) means that aminoacetic acid, more commonly called glycine, is achiral. The other 19 "essential" or "common" amino acids possess sidechains attached in a stere-ochemically identical fashion.

The other 19 common α -amino acids have side chains attached at the position represented by R. Among these 19, proline is unique because its sidechain is attached at the other end to the amino nitrogen, which is therefore secondary rather than primary.

The twenty common α -amino acids may be named systematically. For example, when R is methyl, the compound may be called 2-methylaminoacetic acid. It may also correctly be called 2-aminopropanoic acid. By far, however, it is most commonly called alanine.

TABLE 1.13

Common	IUPAC	IUB	—рКсоон	—pK _{NH3} ⁺	$pK_{Side\ chain}$	I_{pH}	
Alanine	Ala	A	2.34	9.69	_	6.01	H ₃ C OH
Arginine	Arg	R	2.17	9.04	12.84	10.76	NH H ₂ N H H NH ₂ OH
Asparagine	Asn	N	2.02	8.60	_	5.41	H ₂ N OH OH

TABLE 1.13 (continued)

Common	IUPAC	IUB	—pК _{соон}	—рК _{NН3} +	$pK_{Side chain}$	I_{pH}	
Aspartic acid	Asp	D	1.88	9.60	3.65	2.77	HO OH OH
Cystine	Cys	С	1.71	8.18	10.28	5.02	HS OH
Glutamic acid	Glu	E	2.16	9.67	4.32	3.24	HO OH
Glutamine	Gln	Q	2.17	9.13	_	5.65	H ₂ N OH
Glycine	Gly	G	2.34	9.60	_	5.97	H ₂ N OH
Histidine	His	Н	1.82	9.17	6.00	7.59	H OH
Isoleucine	Ile	I	2.36	9.68	_	6.02	H ₃ C OH
Leucine	Leu	L	2.36	9.60	_	5.98	H ₃ C OH
Lysine	Lys	K	2.18	9.12	10.53	9.82	H ₂ N OH
Methionine	Met	M	2.28	9.21	_	5.74	H ₃ C S OH
Phenylalanine	Phe	F	1.83	9.13	_	5.84	OH H NH ₂
Proline	Pro	Р	1.99	10.6	_	6.30	O OH
Serine	Ser	S	2.21	9.15	_	5.68	HO OH

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TABLE 1.13 (continued)

Common	IUPAC	IUB	—рК _{соон}	—pK _{NH3} +	pK Side chain	I_{pH}	
Threonine	Thr	Т	2.71	9.62	_	6.16	H ₃ C OH OH OH NH ₂
Tryptophan	Trp	W	2.38	9.39	_	5.89	HN OH NH2
Tyrosine	Tyr	Y	2.20	9.11	10.07	5.66	HO H NH ₂
Valine	Val	V	2.32	9.62	_	5.96	H ₃ C OH

The names and structures of the twenty natural amino acids are given in Table 1.13. The International Union of Pure and Applied Chemistry (IUPAC) uses the three-letter abbreviations shown in the second column of Table 1.13 to describe amino acids. These are widely used in biological circles as well but are inappropriate when long peptide or protein sequences need to be described. For example, when proinsulin is cleaved, it forms the biologically important peptide insulin and another peptide usually called C-peptide. The human peptide consists of a linear chain of 31 amino acids that have the sequence, from amino to carboxyl, H₂N-Glu-Ala-Glu-Asp-Leu-Gln-Val-Glu-Glu-Glu-Leu-Gly-Gly-Pro-Gly-Ala-Gly-Ser-Leu-Gln-Pro-Leu-Ala-Leu-Glu-Gly-Ser-Leu-Gln-OH. This is readily comprehensible to most chemists because the abbreviations are typically the first three letters of the amino acid. Thus, alanine is Ala and arginine is Arg. Aspartic acid and asparagine cannot both be named Asp so the latter is distinguished as Asn.

Biologists often must compare peptides or proteins from different species. If the IUPAC nomenclature was used, the descriptor for this peptide would be about four-fold longer than if the International Union of Biology's (IUB) single-letter codes are used. Where possible, the first letter of the amino acid's name is used. As with the three-letter abbreviations, this is not always possible. Alanine is A and aspartic acid is arbitrarily assigned the letter D. Asparagine is called N. Glycine is G so glutamic acid is designated E. Although arbitrary, the name is logical for the homologue of aspartic acid. Glutamine is called Q. Arginine cannot use "A," which is taken by alanine, but the letter "R" is suggestive and serves as a mnemonic.

When the single-letter abbreviations are used, the human C-peptide sequence reduces to EAEDLQVGQVELGGGPGAGSLQPLALEGSLQ, often written in groups of five letters as EAEDLQVGQVELGGG PGAGS LQPLA LEGSL Q so that the sequence can be more conveniently read and compared with other sequences.

Most of three-letter abbreviations are taken from the first three letters of the name of the corresponding amino acid and are pronounced as written (alanine-Ala, cysteine-Cys). The one-letter symbol for the amino acids is usually the first letter of the amino acid's name and is often used when comparing the amino acids sequences of several similar proteins.

Note that the single-letter abbreviations permit a fast comparison of the sequences so that their differences and similarities can quickly be discerned. The sequences for C-peptides from humans and from rats are compared below (differences are highlighted):

EAEDL QVGQV ELGGG PGAGS LQPLA LEGSL Q (Human) EVEDP QVPQL ELGGG PEAGD LQTLA LEVAR Q (Rat)

Ten of the amino acids in each sequence differ. Thus, 21 of the 31 amino acids are identical within the sequence. The sequence homology is said to be $(21/31 \times 100) = 68\%$. It would have been much more difficult to make this comparison using the longer three-letter abbreviations. For a protein having 200 or 300 amino acids, the problem becomes correspondingly greater.

Despite the greater economy of using single letter amino acid abbreviations, it is the three-letter abbreviations that have become shortened names for the essential amino acids. For example, practicing scientists would identify the sequence GPAGW as "Gly-Pro-Ala-Gly-Try." A sequence containing both aspartic acid and asparagine such as GAGE would be referred to in conversation as "Gly-Asp-Gly-Asparagine."

Formally, however, the amino acids contained either in peptides or proteins are named

Formally, however, the amino acids contained either in peptides or proteins are named in a fashion related to that used for alkanes. The "-ine" suffix is replaced by "-yl" to give, for GAG, glycyl-alanyl-glycine. Peptide and protein sequences are always written and named from the N-terminus to the C-terminus. The C-terminal amino acid retains its full name.

Stereochemistry

Concepts in stereochemistry, that is, chemistry in three-dimensional space, are in the process of rapid expansion. This section will deal with only the main principles. The compounds discussed will be those that have identical molecular formulas but differ in the arrangement of their atoms in space. *Stereoisomers* is the name applied to these compounds.

Stereoisomers can be grouped into three categories: (1) Conformational isomers differ from each other only in the way their atoms are oriented in space, but can be converted into one another by rotation about sigma bonds. (2) Geometric isomers are compounds in which rotation about a double bond is restricted. (3) Configurational isomers differ from one another only in configuration about a chiral center, axis, or plane. In subsequent structural representations, a broken line denotes a bond projecting behind the plane of the paper and a wedge denotes a bond projecting in front of the plane of the paper. A line of normal thickness denotes a bond lying essentially in the plane of the paper.

Conformational Isomers. A molecule in a conformation into which its atoms return spontaneously after small displacements is termed a *conformer*. Different arrangements of atoms that can be converted into one another by rotation about single bonds are called *conformational isomers* (see Figure 1.3). A pair of conformational isomers can be but do not have to be mirror images of each other. When they are not mirror images, they are called *diastereomers*.

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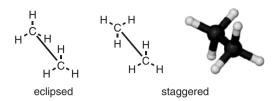


FIGURE 1.3 Eclipsed (left) and staggered (right) conformations of ethane. The ball and stick model is in the staggered conformation.

Acyclic Compounds. Different conformations of acyclic compounds are best viewed by construction of ball-and-stick molecules or by use of Newman projections. Both types of representations are shown for ethane. Atoms or groups that are attached at opposite ends of a single bond should be viewed along the bond axis. If two atoms or groups attached at opposite ends of the bond appear directly one behind the other, these atoms or groups are described as eclipsed. That portion of the molecule is described as being in the eclipsed conformation. If not eclipsed, the atoms or groups and the conformation may be described as staggered. Newman projections show these conformations clearly.

Certain physical properties show that rotation about the single bond is not quite free. For ethane there is an energy barrier of about $3 \, \text{kcal} \cdot \text{mol}^{-1} \, (12 \, \text{kJ} \cdot \text{mol}^{-1})$. The potential energy of the molecule is at a minimum for the staggered conformation, increases with rotation, and reaches a maximum at the eclipsed conformation. The energy required to rotate the atoms or groups about the carbon–carbon bond is called *torsional energy*. Torsional strain is the cause of the relative instability of the eclipsed conformation or any intermediate skew conformations.

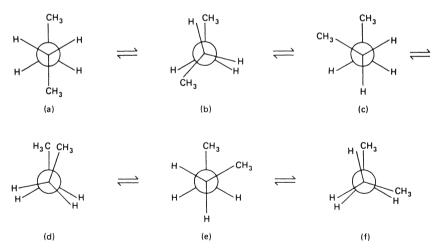


FIGURE 1.4 Conformations of butane. (a) Anti-staggered; (b) eclipsed; (c) gauche-staggered; (d) eclipsed; (e) gauche-staggered; (f) eclipsed. (Eclipsed conformations are slightly staggered for convenience in drawing; actually they are superimposed.)

In butane, with a methyl group replacing one hydrogen on each carbon of ethane, there are several different staggered conformations (see Figure 1.4). There is the *anti* conformation in which the methyl groups are as far apart as they can be (dihedral angle of 180°). There are two *gauche* conformations in which the methyl groups are only 60° apart; these are two nonsuperimposable mirror images of each other. The *anti* conformation is more stable than the *gauche* by about $0.9 \, \text{kcal} \cdot \text{mol}^{-1}$ ($4 \, \text{kJ} \cdot \text{mol}^{-1}$). Both are free of torsional strain. However, in a *gauche* conformation the methyl groups are closer together than the sum of their van der Waals' radii. Under these conditions van der Waals' forces are repulsive and raise the energy of conformation. This strain can affect not only the relative stabilities of various staggered conformations but also the heights of the energy barriers between them. The energy maximum (estimated at 4.8– $6.1 \, \text{kcal} \cdot \text{mol}^{-1}$ or 20– $25 \, \text{kJ} \cdot \text{mol}^{-1}$) is reached when two methyl groups swing past each other (the eclipsed conformation) rather than past hydrogen atoms.

Cyclic Compounds. Although cyclic aliphatic compounds are often drawn as if they were planar geometric figures (a triangle for cyclopropane, a square for cyclobutane, and so on), their structures are not that simple. Cyclopropane does possess the maximum angle strain if one considers the difference between a tetrahedral angle (109.5°) and the 60° angle of the cyclopropane structure. Nevertheless the cyclopropane structure is thermally quite stable. The highest electron density of the carbon–carbon bonds does not lie along the lines connecting the carbon atoms. Bonding electrons lie principally outside the triangular internuclear lines and result in what are known as *bent bonds* (see Figure 1.5).

Cyclobutane has less angle strain than cyclopropane (only 19.5°). It is also believed to have some bent-bond character associated with the carbon–carbon bonds. The molecule exists in a nonplanar conformation in order to minimize hydrogen–hydrogen eclipsing strain.

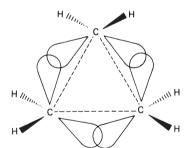


FIGURE 1.5 The bent bonds ("tear drops") of cyclopropane.



FIGURE 1.6 The conformations of cyclopentane.

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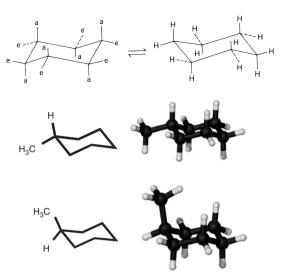


FIGURE 1.7 The two chair conformations of cyclohexane: a = axial hydrogen atom and e = equatorial hydrogen atom. The middle and bottom panels show methylcyclohexane in the chair form with the methyl group equatorial (middle) and axial (bottom).

Cyclopentane is nonplanar, with a structure that resembles an envelope (see Figure 1.6). Four of the carbon atoms are in one plane, and the fifth is out of that plane. The molecule is in continual motion so that the out-of-plane carbon moves rapidly around the ring.

The 12 hydrogen atoms of cyclohexane do not occupy equivalent positions. In the chair conformation six hydrogen atoms are perpendicular to the average plane of the molecule and six are directed outward from the ring, slightly above or below the molecular plane (see Figure 1.7). Bonds which are perpendicular to the molecular plane are known as axial bonds, and those which extend outward from the ring are known as equatorial bonds. The three axial bonds directed upward originate from alternate carbon atoms and are parallel with each other; a similar situation exists for the three axial bonds directed downward. Each equatorial bond is drawn so as to be parallel with the ring carbon-carbon bond once removed from the point of attachment to that equatorial bond. At room temperature, cyclohexane is interconverting rapidly between two chair conformations. As one chair form converts to the other, all the equatorial hydrogen atoms become axial and all the axial hydrogens become equatorial. The interconversion is so rapid that all hydrogen atoms on cyclohexane can be considered equivalent. Interconversion is believed to take place by movement of one side of the chair structure to produce the twist boat, and then movement of the other side of the twist boat to give the other chair form. The chair conformation is the most favored structure for cyclohexane. No angle strain is encountered since all bond angles remain tetrahedral. Torsional strain is minimal because all groups are staggered.

In the boat conformation of cyclohexane (Figure 1.8) eclipsing torsional strain is significant, although no angle strain is encountered. Nonbonded interaction between the two hydrogen atoms across the ring from each other (the "flagpole" hydrogens) is unfavorable. The boat conformation is about $6.5 \, \text{kcal} \cdot \text{mol}^{-1}$ (27 kJ · mol⁻¹) higher in energy than the chair form at 25 °C.

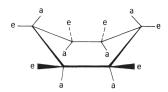


FIGURE 1.8 The boat conformation of cyclohexane. a = axial hydrogen atom and e = equatorial hydrogen atom.

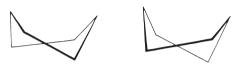


FIGURE 1.9 Twist-boat conformation of cyclohexane.

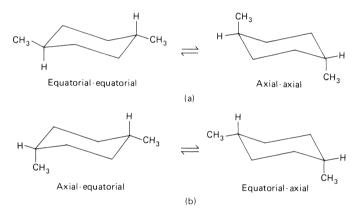


FIGURE 1.10 Two isomers of 1,4-dimethylcyclohexane. (a) Trans isomer; (b) cis isomer.

A modified boat conformation of cyclohexane, known as the twist boat (Figure 1.9), or skew boat, has been suggested to minimize torsional and nonbonded interactions. This particular conformation is estimated to be about $1.5\,\mathrm{kcal}\cdot\mathrm{mol}^{-1}$ (6kJ mol⁻¹) lower in energy than the boat form at room temperature.

The medium-size rings (7-12 ring atoms) are relatively free of angle strain and can easily take a variety of spatial arrangements. They are not large enough to avoid all nonbonded interactions between atoms.

Disubstituted cyclohexanes can exist as *cis-trans* isomers as well as axial-equatorial conformers. Two isomers are predicted for 1,4-dimethylcyclohexane (see Figure 1.10). For the *trans* isomer the diequatorial conformer is the energetically favorable form. Only one *cis* isomer is observed, since the two conformers of the *cis* compound are identical. Interconversion takes place between the conformational (equatorial-axial) isomers but not configurational (*cis-trans*) isomers.

The bicyclic compound decahydronaphthalene, or bicyclo[4.4.0]decane, has two fused six-membered rings. It exists in *cis* and *trans* forms (see Figure 1.11), as determined by the configurations at the bridgehead carbon atoms. Both *cis*- and *trans*-decahydronaphthalene can be constructed with two chair conformations.

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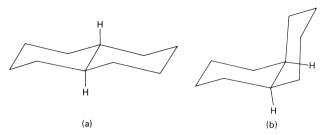


FIGURE 1.11 Two isomers of decahydronaphthalene, or bicyclo[4.4.0]decane. (a) *Trans* isomer; (b) cis isomer.

$$CH_3$$
 $C = C$
 H
 CH_3
 CH

FIGURE 1.12 Two isomers of 2-butene. (a) Cis isomer, bp 3.8° C, mp -138.9° C, dipole moment 0.33 D; (b) trans isomer, bp 0.88° C, mp -105.6° C, dipole moment 0 D.

Geometrical Isomerism. Rotation about a carbon–carbon double bond is restricted because of interaction between the p orbitals which make up the pi bond. Isomerism due to such restricted rotation about a bond is known as *geometric isomerism*. Parallel overlap of the p orbitals of each carbon atom of the double bond forms the molecular orbital of the pi bond. The relatively large barrier to rotation about the pi bond is estimated to be nearly $63 \, \text{kcal} \cdot \text{mol}^{-1}$ ($263 \, \text{kJ} \cdot \text{mol}^{-1}$).

When two different substituents are attached to each carbon atom of the double bond, *cis-trans* isomers can exist. In the case of *cis-2*-butene (Figure 1.12*a*), both methyl groups are on the same side of the double bond. The other isomer has the methyl groups on opposite sides and is designated as *trans-2*-butene (Figure 1.12*b*). Their physical properties are quite different. Geometric isomerism can also exist in ring systems; examples were cited in the previous discussion on conformational isomers.

For compounds containing only double-bonded atoms, the reference plane contains the double-bonded atoms and is perpendicular to the plane containing these atoms and those directly attached to them. It is customary to draw the formulas so that the reference plane is perpendicular to that of the paper. For cyclic compounds the reference plane is that in which the ring skeleton lies or to which it approximates. Cyclic structures are commonly drawn with the ring atoms in the plane of the paper.

Sequence Rules for Geometric Isomers and Chiral Compounds. Although *cis* and *trans* designations have been used for many years, this approach becomes useless in complex systems. To eliminate confusion when each carbon of a double bond or a chiral center is

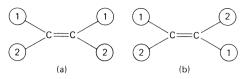


FIGURE 1.13 Configurations designated by priority groups. (a) Z (cis); (b) E (trans).

connected to different groups, the Cahn, Ingold, and Prelog system for designating configuration about a double bond or a chiral center has been adopted by IUPAC. Groups on each carbon atom of the double bond are assigned a first (1) or second (2) priority. Priority is then compared at one carbon relative to the other. When both first priority groups are on the *same side* of the double bond, the configuration is designated as *Z* (from the German *zusammen*, "together"), which was formerly *cis*. If the first priority groups are on *opposite sides* of the double bond, the designation is *E* (from the German *entgegen*, "in opposition to"), which was formerly *trans*. (See Figure 1.13.)

When a molecule contains more than one double bond, each E or Z prefix has associated with it the lower-numbered locant of the double bond concerned. Thus (see also the rules that follow)

When the sequence rules permit alternatives, preference for lower-numbered locants and for inclusion in the principal chain is allotted as follows in the order stated: *Z* over *E* groups and *cis* over *trans* cyclic groups. If a choice is still not attained, then the lower-numbered locant for such a preferred group at the first point of difference is the determining factor. For example,

RULE 1. Priority is assigned to atoms on the basis of atomic number. Higher priority is assigned to atoms of higher atomic number. If two atoms are isotopes of the same element, the atom of higher mass number has the higher priority. For example, in 2-butene, the carbon atom of each methyl group receives first priority over the hydrogen atom connected to the same carbon atom. Around the asymmetric carbon atom in chloroiodomethanesulfonic acid, the priority sequence is I, Cl, S, H. In 1-bromo-1-deuteroethane, the priority sequence is Cl, C, D, H.

RULE 2. When atoms attached directly to a double-bonded carbon have the same priority, the second atoms are considered and so on, if necessary, working outward once again from the double bond or chiral center. For example, in 1-chloro-2-methylbutene, in CH₃ the second atoms are H, H, H and in CH₂CH₃ they are C, H, H. Since carbon has a higher atomic number than hydrogen, the ethyl group has the next highest priority after the chlorine atom.

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CI
$$CH_2CH_3$$
 CI CH_3

C=C

H CH_3
 $C=C$

H CH_2CH_3
 $C=C$
 CH_2CH_3
 $C=C$
 CH_2CH_3
 $C=C$
 CH_3
 C

RULE 3. When groups under consideration have double or triple bonds, the multiplebonded atom is replaced conceptually by two or three single bonds to that same kind of

bonded atom is replaced conceptually by two or three single bonds to that same kind of atom. Thus, =A is considered to be equivalent to two A's, or
$$A$$
 and A are equals A . However, a real A has priority over =A; likewise a real A has priority over A . Actually, both atoms of a multiple bond are duplicated, or triplicated, so that A are treated as A and A has priority over A has priority over A and A has priority over A and A has priority over A and A has priority over A has priority over A and A has priority over A has

atoms themselves are duplicated, not the atoms or groups attached to them. The duplicated atoms (or phantom atoms) may be considered as carrying atomic number zero. For example, among the groups OH, CHO, CH₂OH, and H, the OH group has the highest priority, and the C(O, O, H) of CHO takes priority over the C(O, H, H) of CH₂OH.

Chirality and Optical Activity. A compound is chiral (the term *dissymmetric* was formerly used) if it is not superimposable on its mirror image. A chiral compound does not have a plane of symmetry. Each chiral compound possesses one (or more) of three types of chiral element, namely, a chiral center, a chiral axis, or a chiral plane.

Chiral Center. The chiral center, which is the chiral element most commonly met, is exemplified by an asymmetric carbon with a tetrahedral arrangement of ligands about the carbon. The ligands comprise four different atoms or groups. One "ligand" may be a lone pair of electrons; another, a phantom atom of atomic number zero. This situation is encountered in sulfoxides or with a nitrogen atom. Lactic acid is an example of a molecule with an asymmetric (chiral) carbon. (See Figure 1.14.)

A simpler representation of molecules containing asymmetric carbon atoms is the Fischer projection, which is shown here for the same lactic acid configurations. A Fischer

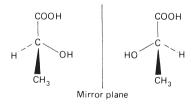


FIGURE 1.14A Stereo drawing of the lactic acid molecule.

FIGURE 1.14B Fischer projection of the lactic acid molecule.

projection involves drawing a cross and attaching to the four ends the four groups that are attached to the asymmetric carbon atom. The asymmetric carbon atom is understood to be located where the lines cross. The horizontal lines are understood to represent bonds coming toward the viewer out of the plane of the paper. The vertical lines represent bonds going away from the viewer behind the plane of the paper as if the vertical line were the side of a circle. The principal chain is depicted in the vertical direction; the lowest-numbered (locant) chain member is placed at the top position. These formulas may be moved sideways or rotated through 180° in the plane of the paper, but they may not be removed from the plane of the paper (i.e., rotated through 90°). In the latter orientation it is essential to use thickened lines (for bonds coming toward the viewer) and dashed lines (for bonds receding from the viewer) to avoid confusion.

Enantiomers. Two nonsuperimposable structures that are mirror images of each other are known as *enantiomers*. Enantiomers are related to each other in the same way that a right hand is related to a left hand. Except for the direction in which they rotate the plane of polarized light, enantiomers are identical in all physical properties. Enantiomers have identical chemical properties except in their reactivity toward optically active reagents.

Enantiomers rotate the plane of polarized light in opposite directions but with equal magnitude. If the light is rotated in a clockwise direction, the sample is said to be dextrorotatory and is designed as (+). When a sample rotates the plane of polarized light in a counterclockwise direction, it is said to be levorotatory and is designed as (-). Use of the designations d and l is discouraged.

Specific Rotation. Optical rotation is caused by individual molecules of the optically active compound. The amount of rotation depends upon how many molecules the light beam encounters in passing through the tube. When allowances are made for the length of the tube that contains the sample and the sample concentration, it is found that the amount of rotation, as well as its direction, is a characteristic of each individual optically active compound.

Specific rotation is the number of degrees of rotation observed if a 1-dm tube is used and the compound being examined is present to the extent of 1 g per 100 mL. The density for a pure liquid replaces the solution concentration.

Specific rotation =
$$[\alpha] = \frac{\text{observed rotation (degrees)}}{\text{length (dm)} \times (\text{g/100 mL})}$$

The temperature of the measurement is indicated by a superscript and the wavelength of the light employed by a subscript written after the bracket; for example, $[\alpha]_{590}^{20}$ implies that the measurement was made at 20 °C using 590 nm radiation.

Optically Inactive Chiral Compounds. Although chirality is a necessary prerequisite for optical activity, chiral compounds are not necessarily optically active. With an equal mixture of two enantiomers, no net optical rotation is observed. Such a mixture of enantiomers is said to be *racemic* and is designated as (\pm) and not as dl. Racemic mixtures usually have melting points higher than the melting point of either pure enantiomer.

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A second type of optically inactive chiral compounds, meso compounds, will be discussed next.

Multiple Chiral Centers. The number of stereoisomers increases rapidly with an increase in the number of chiral centers in a molecule. A molecule possessing two chiral atoms should have four optical isomers, that is, four structures consisting of two pairs of enantiomers. However, if a compound has two chiral centers but both centers have the same four substituents attached, the total number of isomers is three rather than four. One isomer of such a compound is not chiral because it is identical with its mirror image; it has an internal mirror plane. This is an example of a diastereomer. The achiral structure is denoted as a meso compound. Diastereomers have different physical and chemical properties from the optically active enantiomers. Recognition of a plane of symmetry is usually the easiest way to detect a meso compound. The stereoisomers of tartaric acid are examples of compounds with multiple chiral centers (see Figure 1.15), and one of its isomers is a meso compound.

Stereochemistry is sometimes harder to discern in ring systems than in open-chained compounds. The smallest ring, cyclopropane, has six equivalent hydrogens, each of which may be substituted. When a substituent such as a methyl group replaces a hydrogen, the molecule remains achiral because a mirror plane is present that bisects the substituted carbon (and its substituent) and the opposite bond. One side of the cyclopropane therefore reflects the other. The presence of a substituent makes the other cyclopropane positions nonequivalent. Thus a second methyl group may be added on the same carbon (opposite side of the ring) or on one of the adjacent carbons on either the same or opposite sides of the ring. Figure 1.16 shows some of these possibilities. *E*-1,2-Dicarboxycyclopropane (a) exists in two distinct forms. They are nonsuperimposable mirror images; *Z*-1,2-Dicarboxycyclopropane (b) has an internal mirror plane and is therefore superimposable on its mirror image. Structure (d) in Figure 1.16 shows a molecular model of this compound. The carboxyl substituents do not appear to reflect each other but recall that they can rotate freely about the single bond.

A cyclic compound that has two differently substituted asymmetric carbons will have $2^2 = 4$ optical isomers. These will consist of pairs of cis and trans enantiomers. When the asymmetric centers have identical substituents, the cis isomer will have an internal reflection plane and is called a meso form. The meso forms of cis-1,2-dicarboxycyclopropane are shown in panels (b) and (d) of Figure 1.16 in a line angle drawing and as a molecular model.

Torsional Asymmetry. Rotation about single bonds of most acyclic compounds is relatively free at ordinary temperatures. There are, however, some examples of compounds in which nonbonded interactions between large substituent groups inhibit free rotation about a sigma bond. In some cases these compounds can be separated into pairs of enantiomers.

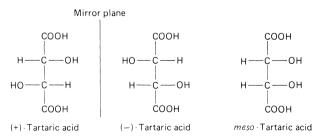


FIGURE 1.15 Isomers of tartaric acid.

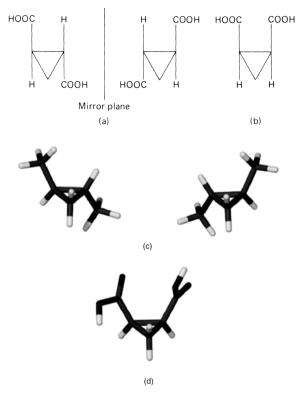
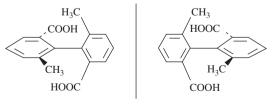


FIGURE 1.16 Isomers of cyclopropane-1,2-dicarboxylic acid. (a) E-1,2-Dicarboxycyclopropane (trans isomers); (b) Z-1,2-Dicarboxycyclopropane isomer. (meso isomer); (c) Molecular models of E-(trans-) 1,2-dimethylcyclopropane shown in the tube representation. Rotation of the right hand structure about a vertical axis through the center of the cyclopropane will superimpose the two methyl groups. The methylene of the rotated structure will be in the back, rather than the front, and not superimposed. (d) A mirror plane through the methylene and the back carboncarbon bond is a plane of symmetry. The two carboxyl groups appear not to reflect each other in the model shown but they can rotate freely and will reflect each other on an instantaneous basis.

A *chiral axis* is present in chiral biaryl derivatives. When bulky groups are located at the *ortho* positions of each aromatic ring in biphenyl, free rotation about the single bond connecting the two rings is inhibited because of torsional strain associated with twisting rotation about the central single bond. Interconversion of enantiomers is prevented (see Figure 1.17).



Mirror plane

FIGURE 1.17 Isomers of biphenyl compounds with bulky groups attached at the *ortho* positions.

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For compounds possessing a chiral axis, the structure can be regarded as an elongated tetrahedron to be viewed along the axis. In deciding upon the absolute configuration it does not matter from which end it is viewed; the nearer pair of ligands receives the first two positions in the order of precedence (see Figure 1.18). For the meaning of (S), see the discussion under "Absolute Configuration".

A *chiral plane* is exemplified by the plane containing the benzene ring and the bromine and oxygen atoms in the chiral compound shown in Figure 1.19. Rotation of the benzene ring around the oxygen-to-ring single bonds is inhibited when *x* is small (although no critical size can be reasonably established).

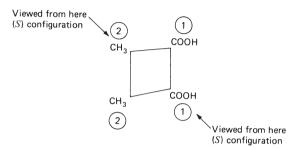


FIGURE 1.18 Example of a chiral axis.

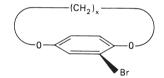


FIGURE 1.19 Example of a chiral plane.

Absolute Configuration. The terms absolute stereochemistry and absolute configuration are used to describe the three-dimensional arrangement of substituents around a chiral element. A general system for designating absolute configuration is based upon the priority system and sequence rules. Each group attached to a chiral center is assigned a number, with number one the highest-priority group. For example, the groups attached to the chiral center of 2-butanol (see Figure 1.20) are assigned these priorities: 1 for OH, 2 for CH₂CH₃, 3 for CH₃, and 4 for H. The molecule is then viewed from the side opposite the group of lowest priority (the hydrogen atom), and the arrangement of the remaining groups are noted. If, in proceeding from the group of highest priority to the group of second priority and

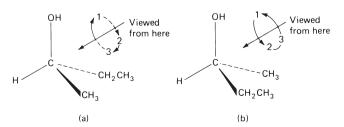


FIGURE 1.20 Viewing angle as a means of designating the absolute configuration of compounds with a chiral axis. (a) (R)-2-butanol (sequence clockwise); (b) (S)-2-butanol (sequence counterclockwise).

thence to the third, the eye travels in a clockwise direction, the configuration is specified R (from the Latin *rectus*, "right"); if the eye travels in a counterclockwise direction, the configuration is specified S (from the Latin *sinister*, "left"). The complete name includes both configuration and direction of optical rotation, as for example, (S)-(+)-2-butanol.

The relative configurations around the chiral centers of many compounds have been established. One optically active compound is converted to another by a sequence of chemical reactions which are stereospecific; that is, each reaction is known to proceed spatially in a specific way. The configuration of one chiral compound can then be related to the configuration of the next in sequence. In order to establish absolute configuration, one must carry out sufficient stereospecific reactions to relate a new compound to another of known absolute configuration. Historically the configuration of D-(+)-2,3-dihydroxypropanal has served as the standard to which all configuration has been compared. The absolute configuration assigned to this compound has been confirmed by an X-ray crystallographic technique.

Stereochemistry in Biological Systems. Amino acids occur naturally in both D and L (*R* and *S*) enantiomeric configurations. Amino acids that occur in proteins almost always have the L configuration although amino acids that occur in bacterial peptides may have the enantiomeric D configuration. The two configurations are shown in Figure 1.21 for alanine.

The description of α -amino acids as D or L is a holdover from an older nomenclature system. In this system (S)-alanine is called L-alanine. The enantiomer would be D- or (R)-serine. The L (laevo, turned to the left; D = dextro, turned to the right) designation refers to the α -carbon in the essential amino acids. In alanine, there is a single α -carbon that is asymmetric. When two asymmetric centers are present as in L-threonine, the stereochemistry of both carbons must be considered. The common form of L-threonine is the 2S.3R stereoisomer.

Threonine (center) is shown in Figure 1.22 along with the simplest chiral amino acid, alanine. The only cyclic amino acid, proline, is pictured as well in the common L-configuration.

Extended Arrangements of Peptides and Proteins. Amino acids are linked from the carboxyl to the amine with formation of an amide bond, often referred to as the peptide link. The repeating (—N—C—CO—) unit is called the peptide or protein backbone. Peptides and proteins differ only in the number of amino acids present in the biopolymer chain. The cutoff is arbitrarily set. Often, but not always, a peptide is designated as having fewer than 100 amino acids and the protein possesses more. Backbone amide groups have been found to play a role in enzyme catalysis.

FIGURE 1.21 Stereochemistry of α -amino acids. The most common, L configuration is shown at the left.

FIGURE 1.22 Structures of alanine, threonine, and proline.

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The extended chains, that is, the backbones, may further organize into assemblies that have characteristic properties. The two most important of these are the α - helix and the β -sheet. The latter is illustrated in Figure 1.23. Panel (a) shows the extensive hydrogen bond organization of peptide chains that are oriented in opposite directions. The arrows indicate the nitrogen to carbonyl (arrowhead) direction. The lower panel (b) shows an alternate H-bond organization when the two peptide chains are parallel rather than antiparallel.

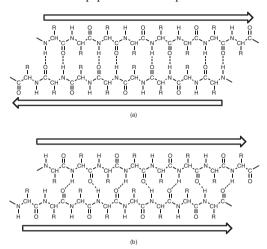


FIGURE 1.23 Hydrogen bonded interactions of peptide chains to form β -sheets. The chains are arranged antiparallel in panel (a) and parallel in panel (b).

An alternate organization for peptide chains is the α -helix. It is essentially a coil in which a carbonyl group H-bonds an amide nitrogen between every fourth residue. The resulting structure exhibits one full turn for each 3.6 amino acids, which spans 5.4 Å per turn. The resulting α -helix is a tight coil that lacks any significant interior space. A schematic representation of the H-bonded coil is shown in Figure 1.24.

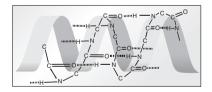


FIGURE 1.24

A number of other arrangements are possible for peptide or protein chains. A discussion of them is beyond the scope of this Handbook.

Chemical Abstracts Indexing System

When compounds of complex structure are considered, the number of name possibilities grows rapidly. To avoid having index entries for all possible names, Chemical Abstracts Service has developed what might be called the principle of inversion. The indexing system employs inverted entries to bring together related compounds in an alphabetically arranged index. The *index heading parent* from the Chemical Substance Index appears in the Formula Index in lightface before the "comma of inversion." The *substituents* follow the "comma of

inversion" in alphabetical order. Any *name modificat* ion appears on a separate line. If necessary, the chemical description is completed by citation of an associated ion, a functional derivative, a "salt with" or "compound with" terms and/or a stereochemical descriptor.

Quite naturally there is a certain amount of arbitrariness in this system, although the IUPAC nomenclature is followed. The preferred *Chemical Abstracts* index names for chemical substances have been, with very few exceptions, continued unchanged (since 1972) as set forth in the *Ninth Collective Index Guide* and in a journal article.* Any revisions appear in the updated *Index Guide*; new editions appear at 18-month intervals. Appendix VI is of particular interest to chemists. Reprints of the Appendix may be purchased from Chemical Abstracts Service, Marketing Division, P.O. Box 3012, Columbus, Ohio 43210.

PHYSICAL PROPERTIES OF PURE SUBSTANCES

TABLE 1.14 Empirical Formula Index for Organic Compounds

The alphanumeric designations are keyed to Table 1.15

Cl ₂ H ₂ Si: d226	CH ₂ Cl ₂ : d190	CH ₄ S: m33
Cl ₃ HSi: t247	CH ₂ Cl ₄ Si: c165	CH ₅ AsO ₃ : m125
Cl ₆ OSi ₂ : h28	CH ₂ I ₂ : d404	CH ₅ N: m115
	CH ₂ N ₂ : c285, d47	CH ₅ NO ₃ S: a205
C_1	CH ₂ N ₄ : t136	CH ₅ N ₃ : g29
	CH ₂ O: f27	CH ₅ N ₃ O: s3
	(CH ₂ O) _x : p1	CH ₅ N ₃ S: t162
CBrClF ₂ : b255	CH ₂ O ₂ : f32	CH ₆ N ₂ : m270
CBrCl ₃ : b358	CH ₂ S ₃ : t434	CH ₆ N ₄ : a180, a181
CBrF ₃ : b360	CH ₃ Br: b300	CH ₆ N ₄ O: c11
CBr_2F_2 : d75	CH ₃ Br ₃ Ge: m254	CN ₄ O ₈ : t126a
CClF ₃ : c253	CH ₃ Cl: c137	
CCINO ₃ S: c240	CH ₃ ClHg: m295	C ₂
CCl_2F_2 : d170	CH ₃ ClO ₂ S: m32	
CCl ₃ D: c127	CH ₃ Cl ₃ Ge: m437	
CCl ₃ F: t232	CH ₃ Cl ₃ Si: t238	$C_2Br_2ClF_3$: d72
CCl ₃ NO ₂ : t239	CH ₃ DO: m35	$C_2Br_2Cl_4$: d99
CCl ₄ O ₂ S: t236	CH ₃ F: f18	$C_2Br_2F_4$: d100
CCl ₄ S: t235	CH ₃ I: i40	$C_2Br_2O_2$: o50
CD ₄ O: m36	CH ₃ NO: f28	C ₂ ClF ₃ : c252
CHBrCl ₂ : b266	CH ₃ NO ₃ : m314, n56	$C_2Cl_2F_3I$: d188
CHBr ₂ Cl: d71	CH ₃ NO ₃ : m313	$C_2Cl_2F_4$: d227
CHBr ₃ : t206	CH ₃ N ₅ : a289	$C_2Cl_2O_2$: o51
CHClF ₂ : c85	CH₄: m29	$C_2Cl_3F_3$: t251
CHCl ₂ F: d183	CH ₄ Cl ₂ Si: d199, m222	C ₂ Cl ₃ N: t217
CHCl ₃ : c126	CH ₄ N ₂ O: f34, u12	C ₂ Cl ₄ : t29
CHF ₃ : t295	CH ₄ N ₂ O ₂ S: f30	C ₂ Cl ₄ F ₂ : d347, d348, t26
CHF ₃ O ₃ S: t296	CH ₄ N ₂ S: t163	C ₂ Cl ₄ O: t218
CHI ₃ : i36	CH ₄ N ₄ O ₂ : n54	C ₂ Cl ₆ : h29
CHN ₃ O ₆ : t385	CH ₄ O: m34	$C_2D_3N: a30$
CH ₂ BrCl: b256	CH ₄ O ₂ : m275	$C_2D_4O_2$: a21
CH ₂ Br ₂ : d88	$CH_4O_3S: m30$	$C_2D_6OS: d615$

^{*}J. Chem. Doc., 14(1): 3-15 (1974).

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to table 1.15

 $C_{2}F_{4}$: t63 C₂F₆: h44 $C_{2}F_{6}O_{5}S_{2}$: t297 C2HBrClF3: b258 $C_2HBr_2F_3$: d103 C₂HBr₂N: d63 C₂HBr₃: t205 C2HBr3O: t201 C2HBr3O2: t202 C2HClF2O2: c83 C2HCl2F3: d232 C2HCl3: t230 C2HCl3O: d141 C2HCl3O2: t216 C2HCl5: p9 C₂HF₃O₂: t287 C₂H₂: a41 C₂H₂BrClO: b224 $C_2H_2Br_3$: d80, d81 $C_2H_2Br_2F_2$: d74 C₂H₂Br₂O: b223 $C_2H_2Br_2O_2$: d62 C2H2Br4: t9 C₂H₂ClF₃: c251 C₂H₂ClN: c27 C₂H₂Cl₂: d178, d179, d180 C₂H₂Cl₂O: c31 C2H2Cl2O2: d138 C₂H₂Cl₄: t27, t28 C₂H₂F₃NO: t286 C₂H₂O: k1 C₂H₂O₂: g27 C₂H₂O₃: g28 C₂H₂O₄: o48, o49 C₂H₃Br: b284 C₂H₃BrO: a35 C₂H₃BrO₂: b220 C₂H₃Br₂Cl₃Si: d82 C₂H₃Br₃O: t204 C₂H₃Cl: c109 C₂H₃ClF₂: c84 C₂H₃ClO: a37 C₂H₃ClO₂: c24, m187 C₂H₃Cl₃: t226, t227 C₂H₃Cl₃O: t228 C2H3Cl3Si: t252

C₂H₃Cl₅Si: d182 C₂H₃DO₂: a20 C₂H₃FO: a43 C₂H₃FO₂: f6 C₂H₃F₃: t291 C₂H₂F₂O: t292 C₂H₃IO: a48 C2H3IO2: i25 C₂H₃N: a29 C₂H₃NO: m287 C2H3NS: m289, m426 C2H3N3: t199 C₂H₃N₃S₂: a290 C2H4BrCl: b254 C₂H₄BrNO: b218 C₂H₄Br₂: d77, d78 C2H4CINO: c22 C₂H₄Cl₂: d176, d177 C₂H₄Cl₂O: d197 C₂H₄Cl₆Si₂: b204 C₂H₄FNO: f5 $C_2H_4F_2$: d346 C2H4INO: i24 C₂H₄I₂: d403 C₂H₄N₂: a106 C₂H₄N₂O₂: o54 C2H4N2O4: d632 C₂H₄N₂O₆: e126 C2H4N2S2: d710 C₂H₄N₄: a295, d235 $C_2H_4N_4O_2$: a324 C₂H₄O: a4, e129 C2H4OS: t142 C₂H₄O₂: a19, h86, m250 $C_2H_4O_2S: m14$ C₂H₄O₃: h87, p59 $C_2H_4O_5S: s23$ $C_2H_4S: e130$ C2H5AlCl2: e57 C₂H₅Br: b277 C2H5BrNaO2S: b278 C₂H₅BrO: b279, b308 C2H5C1: c102 C₂H₅ClHg: e165 C₂H₅ClO: c103, c155 C₂H₅ClO₂S: e19

C₂H₅Cl₂OPS: e117 C₂H₅Cl₂O₂P: e116 C₂H₅Cl₃Si: c153, t231 C2H5DO: e22 C2H5F: f17 C2H5FO3S: e134 C₂H₅I: i34 C₂H₅IO: i35 C2H5N: e131 C₂H₅NO: a5, a6, m248 C₂H₅NO₂: e186, g25, m181, n53 C₂H₅NO₃: e185 C2H5NS: t141 C₂H₅N₃O₂: b215, o53 C₂H₆: e14 C₂H₆BrN: b281 C₂H₆Cd: d501 C2H6CIN: c106 C2H6CINO2S: d609 C₂H₆ClO₂PS: d504 C2H6Cl2Si: d174 C₂H₆Hg: d546 $C_2H_6N_2$: a7 C₂H₆N₂O: a25, m444, n79 C₂H₆N₂O₂: m271 $C_2H_6N_2O_4S: a107$ $C_2H_6N_2S: m431$ C₂H₆N₄O₂: o52 C₂H₆O: d518, e21 C₂H₆OS: d614, m18 C₂H₆O₂: e16, e128 C₂H₆O₂S: d613 $C_2H_6O_3S: d612, m297$ C₂H₆O₄S: d610, h114 $C_2H_6O_5S_2$: m31 C₂H₆S: d611, e20 C₂H₆S₂: d516, e18 C₂H₆Te: d617 C₂H₆Zn: d624 C₂H₇AsO₂: d484 C2H2ClSi: c92 C2H2N: d461, e58 C₂H₇NO: a163, a164 C₂H₇NO₃S: a161

C2H5CIS: c156

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

 $\begin{array}{l} C_2H_7NO_4S: a169 \\ C_2H_7NS: a162 \\ C_2H_7N_5: b133 \\ C_2H_7O_3P: d541 \\ C_2H_8N_2: d539, d540, e15 \\ C_2H_8N_2O: h120 \end{array}$

 C_3

 $C_3Br_2F_6$: d85 C₃Cl₃NO₂: t219 C2Cl2N2: t250 C₃Cl₃N₃O₃: t234 C3Cl6: h31 C₃Cl₆O: h23 C₃D₆O: a27 C3HCl5O: p7 C₃H₂CIN: c32 $C_3H_2Cl_2O_2$: m6 C3H2Cl4: t33 C3H2Cl4O: t21 C₃H₂Cl₄O₂: t229 C₃H₂F₆O: h45 $C_3H_2N_2$: m5 C₃H₂N₂O₃: i6 C₃H₂O₂: p241 C₃H₃Br: b344 C₃H₃Cl: c232 C₃H₃ClO: a65 C₃H₃Cl₃O: e13 C₃H₃N: a64 C₃H₃NOS₂: r3 C₃H₃NO₂: c287 C₃H₃NS: t140 C₃H₃N₃O₂S: a249 C₃H₃N₃O₃: c299 C₃H₄: a78, p240 C₃H₄BrClO: b340, b341 C₃H₄BrN: b339 C₃H₄Br₂: d95 $C_3H_4Br_2O_2$: d96 C₃H₄ClN: c220 C₃H₄Cl₂: d221, d222 C₃H₄Cl₂O: c221, c222, d139

C₃H₄Cl₂O₂: m219 C₃H₄Cl₃NO: m436 C₃H₄F₄O: t64 C₃H₄N₂: i4, p245 C₃H₄N₂O: c286 C2H4N2OS: t152 C₃H₄N₂O₂: h84 C₃H₄N₂S: a291 C₃H₄O: p204, p242 $C_3H_4O_2$: a63, o59, p210 C₃H₄O₃: e124, o60 $C_3H_4O_4$: m3 C₃H₅Br: a85, b225, b335, b336 C₂H₅BrO: b276 C₃H₅BrO₂: b337, b338, m143 C₃H₅Br₃: t208 C₃H₅Cl: c216 C₃H₅ClO: c101, c215, p216 C3H5ClOS: e101 C₃H₅ClO₂: c218, c219, e98, m182 C3H5Cl3: t244 C₃H₅Cl₃O: t245 C₃H₅Cl₃Si: a102 C₃H₅FO: f7 C₃H₅F₃O₃S: m438 C₃H₅I: a92, i50 C₃H₅N: p215 C₃H₅NO: a62, c290, h168, h169 C₃H₅NO₂: o55 C₃H₅NS: e161, m421 C₃H₅N₃O: c288 C₃H₅N₃O₉: g21 C₃H₅N₃S: c292 C₃H₆: c364, p205 C₃H₆BrCl: b257 C₃H₆BrNO₄: b316 $C_3H_6Br_2$: d92, d93 C₃H₆Br₂O: d94 C₃H₆ClNO: d502 C₃H₆Cl₂: d218, d219 C₃H₆Cl₂O: d220

C₃H₆Cl₂Si: d200

C₃H₆Cl₄Si: c229 C₃H₆I₂: d405 C₃H₆N₂: a274, d505 C₃H₆N₂O: i7 $C_3H_6N_2O_2$: m4, m269 C2H6N2S: a292, i5 C₃H₆N₂OS: a58 C3H6N6: t198 C₃H₆O: a26, a81, e10, m446, p211, p227, t345 C₃H₆OS: m420, t161 C₃H₆O₂: d647, e11, e135, h89, m111, p213 C₃H₆O₂S: m21, m293 C₃H₆O₃: d397, d398, d503, L1, L2, m38, m259, t388 C₃H₆O₃S: p198 C₃H₆S: p206, p228, t345a C3H6S3: t431 C₂H₇Br: b332, b333 C₃H₇BrO: b334 C₃H₇C1: c210, c211 C₃H₇ClO: c111, c152, c213, c214 C₃H₇ClOS: c136 C3H7ClO3: c212 C₃H₇ClO₂S: p197 C₃H₇Cl₂OP: p236 C₃H₇Cl₃Si: d194, p237 C₃H₇I: i48, i49 C₃H₇N: a82, p226 C₃H₇NO: a28, d522, m110, p212 C₃H₇NO₂: a73, a74, a75, a76, e91, m258, n73, n74 C₃H₇NO₂S: c370 C₃H₇NO₃: i105, n75, p233, C3H7NO5S: a288 C₃H₇NS: d620 C₃H₇NS₂: d517 $C_3H_7O_5P: c17$ C₃H₈: p191 C₃H₈ClN: c224 C₃H₈Cl₂Si: c75, c150

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C2H0IN: d549 C₃H₈N₂O: d623, e230 C₃H₈N₂O₂: e92, f29 C₃H₈N₂S: d621 C₃H₈O: e171, p202, p203 C₃H₈OS₂: d425, m305 C₃H₈O₂: d441, m65, p194, p195 C2H2O2S: m20 C₃H₈O₃: g16 C₃H₈S: e182, p199, p200 C₃H₈S₂: p196 C₃H_oAl: t327 C₃H₈BO₃: t319 C₃H₀B₃O₆: t320 C₃H₉BrGe: b363 C₃H₀BrSi: b364 C2H0ClGe: c254 C₃H₀ClSi: c255 C₂H₀IOS: t378 C₃H₀IS: t377 C2H0ISi: i55 C₃H₀N: i88, m246, p220, t328 C₃H₀NO: a269, a270, a271, a272, m69, m119, t329 C₃H₀NO₂: a268 C2H0N2Si: a319 C₃H₉O₃P: d551, t364 C₃H₉O₄P: t363 C₃H₁₀N₂: m247, p192, p193 $C_3H_{10}N_2O: d43$ C₃H₁₁Br₂N₃S: a171

C_4

C₄Cl₂F₆: d185 C₄Cl₂F₈: d206 C₄Cl₂O₃: d189 C₄Cl₃F₇: h3 C₄Cl₆: h25 C₄D₆O₃: a23 C₄F₆O₃: t288 C₄HBrO₃: b299 C4HCl3N2: t246 $C_4HF_7O_2$: h2 C₄H₂: b376 C4H2Br2S: d101 C₄H₂Cl₂N₂: d223 C₄H₂Cl₂O₂: f38 C₄H₂Cl₂O₃: d208 C₄H₂Cl₂S: d228 $C_4H_2F_6O_2$: t294 $C_4H_2O_3$: m2 C4H2O4: a42 C₄H₃BrS: b353 C₄H₃ClS: c242 C4H3Cl2N3O: d193 C₄H₃IS: i52 C₄H₄: b407 C₄H₄BrNO₂: b351 C₄H₄Br₂O₂: d69 C4H4Br2O4: d98 C₄H₄ClNO₂: c239 C4H4Cl5: d168 $C_4H_4Cl_2O_2$: s19 C₄H₄Cl₂O₂: c25 C₄H₄N₂: b380, p244, p247, p267, s18 $C_4H_4N_2O_2$: d400, p268 C₄H₄N₂O₂S: d388 C4H4N2O3: b1 C₄H₄N₂O₅: a79 $C_4H_4N_4$: d40 C₄H₄O: f40 C₄H₄O₂: d422 C₄H₄O₃: s16 C₄H₄O₄: f37, ml C₄H₄S: t154 $C_4H_5BrO_4$: b350 C₄H₅Cl: c63, c70 C₄H₅ClO: c283, c366, m28 C₄H₅ClO₂: a87 C₄H₅ClO₂: e191 C₄H₅Cl₃O₂: e226 $C_4H_5F_3O_2$: e227 C₄H₅N: b400, c365, m27, p269 C4H5NO: m290

C₄H₅NO₂: e106, m193, s17 C₄H₅NO₂S: e32 C4H5NO3: h182 C₄H₅NS: a93 C₄H₅N₃: a284, i11 C4H5N3O: a198 C₄H₅N₃OS: a191 $C_4H_5N_3O_2$: a154, a155, c289, m322 C₄H₆: b373, b374, b490, b491 $C_4H_6Br_2O_2$: d70 C₄H₆ClN: c73 C₄H₆Cl₂: d165, d166, d167 C4H6Cl2O: c74 $C_4H_6Cl_2O_2$: m220 C₄H₆Cl₃NSi: c294 C₄H₆N₂: a151, m280, m281, m282 C₄H₆N₂O₂: e114 C₄H₆N₂S: a229 C₄H₆N₄O: d39 $C_4H_6N_4O_3$: a77 C₄H₆O: b406, c282, d356, d545a, m24, m396 $C_4H_6O_2$: b386, b401, b402, b403, b492, b497, b498, c367, m26, m114, v2 C4H6O5S: d368 $C_4H_6O_3$: a22, a24, m334, o56, p225 $C_4H_6O_4$: d566, s14 $C_4H_6O_4S: m23, t148$ C₄H₆O₅: h180, h181, o61 $C_4H_6O_6$: t1, t2 C₄H₇Br: b240, b241, b242 $C_4H_7BrO_2$: b244, b280, b307, e75, m146 C₄H₇Cl: c68, c69, c163, C₄H₇ClO: b501, c67, c115, $C_4H_7ClO_2$: c71, c72, e94, m189 C₄H₇Cl₂NSi: c291 $C_4H_7Cl_3O: t237$

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

C4H7Cl3O2Si: c13 C₄H₇FO₅: e133 C₄H₇N: b499, i76 C₄H₇NO: h145, i98, m25, m334, p231, p275 C₄H₇NO₅: m331 C₄H₇NO₃: a46, e192, p12 C₄H₇NO₄: a314, i10 C4H7NS: m419 C₄H₇N₂O: c278 C₄H₈: b395, b396, b397, c300, m383 C₄H₈BrCl: b251 C₄H₈Br₂: d67, d68 C4H8Br2O: b149 C₄H₈Cl₂: d162, d163, d164 C₄H₈Cl₂O: b158, d181 C₄H₆Cl₂Si: a89 C₄H₈N₂O: a105, a150 $C_4H_0N_2O_2$: d526, s13 C₄H₈N₂O₃: a313, g26 C₄H₉N₂S: a101, t79 C₄H₈O: b393, b404, b405, b493, e3, e232, i73, m96, m377, m385, t66 C₄H₈OS: e220, t107, t164 C₄H₈O₂: b398, b399, b495, d646, e51, h106, i75, m389, m390, p229 C₄H₈O₂S: e164, m294, t106 C₄H₆O₂: e23, e150, h116, h127, m64, m291, m298 C4H6O2S: m384 C₄H₈S: a95, t81 $C_4H_8S_5$: d707 C₄H₀Br: b238, b239, b310, b311 C₄H₆BrO: b285 C₄H₉Cl: c64, c65, c161, c162 C₄H₀ClO: c66, c110 C₄H₉ClO₂: c89, c104, m67 C₄H₀ClSi: c93 C₄H₉Cl₃Si: b483, c225 C4H9Cl3Sn: b481

C₄H₆F: f20 C₄H₉I: i30, i31, i43, i44 C₄H₀Li: b457, b458 C₄H₀N: p270 C₄H₀NO: a321, b394, b494, d458, e52, i74, m388, m448 C₄H₉NO₂: a138, a139, a222, b464, b465, h115, i71, n50 C₄H₀NO₂S: a204 C₄H₉NO₃: a187, a188, a189, a190, i70, n51 C₄H₉NSi: c298 C4H9N3O2: c277 C₄H₁₀: b378, m375 C4H10ClN: d467 C4H10ClO2PS: d292 C4H10ClO3P: d291 C₄H₁₀Cl₂Si: b160, m392 $C_4H_{10}N_2$: p179 C4H10N2O: a231 C₄H₁₀N₂O₄S: a8 C₄H₁₀O: b391, b392, d300, m381, m382, m393 C₄H₁₀OS: e153 C₄H₁₀OS₂: b186 C₄H₁₀O₂: b381, b382, b383, b384, b385, b453, d438, d439, e34, m95 $C_4H_{10}O_2S$: m430, t149 $C_4H_{10}O_2S_2$: d424, h118 C₄H₁₀O₃: b181, b390, t351 C4H10O3S: d338 C4H10O4S: d336 C₄H₁₀S: b388, b389, d337, i104, m378, m379, m380, m395 C₄H₁₀S₂: b387, d294a $C_4H_{10}S_3$: b187 C₄H₁₀Zn: d344 C4H11ClSi: c166 C₄H₁₁N: b377, b417, b418, d267, d268, d520, i63 C₄H₁₁NO: a136, a137, a221, d315, d465, e38, e62

C₄H₁₁NO₂: a165, a220, d245, d440 C4H11NO3: t423 C4H11O2PS2: d296 C4H11O3P: d314 C4H12BrN: t93 C4H12ClN: t94 C₄H₁₂Ge: t109 C4H12IN: t95 C₄H₁₂N₂: b379, b452, d521, m376, m377 C4H12N2O: a166 C4H12N2S2: c369 C4H12OSi: m108 C4H12O3Si: t326a C4H12O4Si: t92 C₄H₁₂Pb: t112 C4H12Si: t120 C₄H₁₂Sn: t123 C4H12N2: d298 C4H14OSi2: t105 C4H16O4Si4: t103

C_5

C₅Cl₅N: p12 C₅Cl₆: h27 C₅D₅N: p249 C₅H₃Br₂N: d97 C5H3ClO2: f48 C5H3Cl2N: d224 C₅H₄BrN: b345, b346 C5H4CIN: c233 C₅H₄FN: f23 C₅H₄F₈O: o18 C₅H₄N₂O₃: n76 C5H4N4O: h186 C₅H₄N₄O₃: u13 C₅H₄OS: t156 C5H4O2: f39 C5H4O2S: t157 C₅H₄O₃: c271, f42 C₅H₅ClN₂: a149 C5H5CIN5O5: c167 $C_5H_5F_3O_5$: t293

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₅H₅N: p248 C₅H₅NO: h173, h174, h175, p262 C₅H₅NO₂: d401, h177 C₅H₅NO₃S: p263 C5H5N3O3: a248 C5H5N3O4: a160 C5H5N5: a69 C₅H₆: m166 $C_5H_6Br_2N_2O_3$: d76 C5H6Cl2N2O2: d173 C₅H₆Cl₂O₂: d195, g15 C₅H₆Cl₄O₂: t225 C₅H₆N₂: a281, a282, a283, g14, m397, v7 C₅H₆N₂O: a47, a197 C5H6N2OS: h128 C₅H₆N₂O₂: d391 C₅H₆N₂O₂: e107 C₅H₆O: m59, m252 C₅H₆OS: f44 C₅H₆O₂: f46 C₅H₆O₃: g12 C₅H₆O₄: c270, m245 $C_5H_6O_4S_3$: b155 C₅H₆S: m427 C₅H₇BrO₂: m145 C₅H₇BrO₃: e79 C₅H₇ClO₃: m183, m188 C₅H₇N: m404 C₅H₇NO: f47 C₅H₇NO₂: e105 C₅H₇NS: t158 C₅H₇N₃: a228, d44 C₅H₇N₃O: a192 C_5H_8 : c358, m147, m148, m171, p16, p17, p18, p19, p57 $C_5H_8Br_2O_2$: e115 $C_5H_8Br_4$: p21 C₅H₈F₄O: m414 C₅H₈N₂: d542, d603, e159, p272 C₅H₈N₂O: m449 C5H8N2O2: d538 C₅H₈N₄O₁₂: p22

C₅H₈O: c356, c368, d363, e8, m172, p51 C₅H₈O₂: a80, e56, g13, i84, m58, m161, m162, m163, m192, m217, m296, p31, p32, p40, p40a, p50, p208 C₅H₈O₃: e196, m112, o58 C₅H₈O₄: d545, g11, m274, m412 C₅H₉Br: b263 C₅H₉BrO₂: e81, e82, m144 C₅H₉Cl: c79 C₅H₀ClO: c192, d600, m179, p44 C₅H₀ClOS: b437, c229 C₅H₀ClO₂: b436, e99, e100, i65, m186 C5H0F3O2Si: t376 C₅H₉N: d602, m178, p33, C₅H₀NO: b455, b456, c357, e193, m406 C₅H₉NO₂: m118, p273 C₅H₉NO₄: g9 C₅H₉N₃: i8 C₅H₁₀ c352, m158, m159, m160, p47, p48, p49 $C_5H_{10}Br_2$: d91 C5H10CINO: d288 C₅H₁₀Cl₂: d209 C5H10Cl2O2Si: c12 C5H10Cl2Si: c351 C5H10N2: d293, d474 C₅H₁₀N₂O: d543, p180 $C_5H_{10}N_2O_3$: g10 C₅H₁₀O: a91, c355, d596, i108, m157, m164, m165, m173, m174, m415, p27, p41, p42, t76 C₅H₁₀OS: m425 $C_5H_{10}O_2$: d454, d598, e208, h139, h156, h157, i66, i87, m102, m175, m176, m177, m286, p36, p219, t68

C₅H₁₀O₂S: e183, m306, m417 C₅H₁₀O₃: d289, d451, e162, m68, m278 C5H10O4: b184 $C_5H_{10}O_5$: a310, r5, x8 C₅H₁₁Br: b305, b322, b323 C₅H₁₁BrO₂: b269 C₅H₁₁BrO₂Si: t370 C₅H₁₁Cl: c91, c148, c149, c191 C5H11ClSi: a86 C5H11Cl2N: b159 C₅H₁₁I: i42, i47 C₅H₁₁N: a90, m405, p183 C₅H₁₁NO: d304, d597, h167, m307, t69 C₅H₁₁NO₂: a253, a254, b128, e231, i81, v1 C₅H₁₁NO₂S: m37 C₅H₁₁NO₃: n58 C₅H₁₁NS₂: d295 C₅H₁₁O₅P: t365 C_5H_{12} : d592, m149, p28 C₅H₁₂ClN: d475 C₅H₁₂Cl₂O₂Si: b157 $C_5H_{12}N_2$: a267, m368, m369 C₅H₁₂N₂O: b487, t124 C₅H₁₂N₂O₂: b430, o46 C₅H₁₂N₂S: t122 $C_5H_{12}N_2S_2$: p271 C₅H₁₂O: b460, d452, d595, e209, m153, m154, m155, m156, p37, p38, p39 C5H12OSi: t379 C₅H₁₂O₂: d594, m57, p30 C₅H₁₂O₂S: e221 $C_5H_{12}O_3$: h141, m66, t352, t425 C₅H₁₂O₃S: p34 $C_5H_{12}O_4$: p20, t114 C₅H₁₂O₅: x7 C₅H₁₂S: b463, e210, m150, m151, m152, p35

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

 $\begin{array}{l} C_5H_{12}Si:\ t380 \\ C_5H_{13}N:\ a251,\ a252,\ d601,\\ m167,\ m168,\ m169,\ p53 \\ C_5H_{13}NO:\ a213,\ a214,\\ a255,\ d472,\ d473,\ e47,\\ i89,\ p221 \\ C_5H_{12}NOSi:\ t368 \\ C_5H_{13}NO_2:\ a176,\ d442,\\ d471,\ d523,\ m223 \\ C_5H_{13}N_3:\ t110 \\ C_5H_{14}N_2:\ d593,\ p29,\ t113 \\ C_5H_{14}OSi:\ e50,\ t372 \\ C_5H_{14}O_2Si:\ d255 \\ C_5H_{15}N_3:\ a175 \end{array}$

C_6

C₆BrD₅: b230 C₆BrF₅: b321 C₆Cl₄O₂: t24, t25 C₆Cl₅NO₂: p10 C₆Cl₆: h24 C₆D₆: b10 C_6D_{12} : c313 C₆F₆: h43 C₆HBr₅O: p6 C6HCl4NO2: t30 C5HCl5: p8 C6HCl5O: p11 C₆H₂BrFN₂O₄: b272 C₆H₂Cl₂O₄: d172 C₆H₂Cl₃NO₂: t242a C₆H₂Cl₄: t22, t23 C₆H₃Br₂F: d84 $C_6H_3Br_2NO_2$: d90 C₆H₃Br₃O, t207 C₆H₃ClFNO₂: c121 C₆H₃ClN₂O₄: c94, c95 C₆H₃ClN₂O₄S: d627 C₆H₃Cl₂NO₂: d203, d204, d205 C₆H₃Cl₃: t222, t223, t224 C₆H₂Cl₂O: t240, t241 C6H3Cl3O2S: d155 $C_6H_3FN_2O_4$: d633

C₆H₃N₃O₆: t382, t383 C₆H₃N₃O₇: p173 C₆H₄BrCl: b247, b248, b249 C₆H₄BrClO₂S: b231 C.H.BrF: b288, b289, b290 C₆H₄BrNO₂: b314 C₆H₄BrN₃O₄: b271 C₆H₄Br₂: d65 C₆H₄Br₂N₂O₂: d89 C₆H₄Br₃N: t203 C₆H₄ClF: c116, c117, c118 C₆H₄ClFO: c122 C₆H₄ClI: c135 C₆H₄ClNO₂: c175, c176, c177, c234, c235 C₆H₄ClNO₃: c186 C₆H₄ClNO₄S: n35 C₆H₄ClO₂P: p110 C₆H₄Cl₂: d152, d153, d154 C₆H₄Cl₂N₂O₂: d202 C₆H₄Cl₂O: d210, d211, d212, d213 C6H4Cl2O2: d171 C₆H₄Cl₂O₂S: c43 C₆H₄Cl₃N: t220, t221 C₆H₄Cl₄Si: c208 C₆H₄FNO₂: f21 $C_6H_4F_2$: d345 $C_6H_4INO_2$: i45 C₆H₄I₂: d402 C₆H₄N₂: c295, c296, c297 C₆H₄N₂O₂: b43 C₆H₄N₂O₄: d626 C₆H₄N₂O₅: d635 C₆H₄N₄: a273 $C_6H_4N_4O_6$: t381 C₆H₄O₅: b59 C₆H₅BO₂: c21 C₆H₅Br: b229 C₆H₅BrO: b325, b326 C₆H₅BrS: b354 C₆H₅Cl: c41 C₆H₅ClHg: p126 C₆H₅ClN₂O₂: c172, c173a, c173, c174

C₆H₅ClO: c194, c195, c196 C₆H₅ClO₂: c87, c88 C₆H₅ClO₂S: b23 C₆H₅ClS: c243 C₆H₅ClSe: p151 C₆H₅Cl₂N: d142, d143, d144, d145, d146, d147 C₆H₅Cl₂OP: p137 C₆H₅Cl₂O₂P: p105 C₆H₅Cl₂P: d216 C6H5Cl5PS: p138 C₆H₅Cl₃Si: p155 $C_6H_5D:b9$ C₆H₅F: f11 C₆H₅FO: f22 C₆H₅FO₂S: b24 C₆H₅F₇O₂: e137 C6H5I: i27 C₆H₅NO: n78, p251, p252, p253 C₆H₅NOS: t153 C₆H₅NO₂: n30, n83, p255, p256, p257 C₆H₅NO₃: h176, n60, n61 C₆H₅NO₄: c272 C₆H₅N₂: b62 C₆H₅N₃O: h103 C₆H₅N₃O₄: d625 C₆H₆: b8a C₆H₆AsNO₆: h153 C₆H₆BrN: b225, b226, b227 C₆H₆ClN: c33, c34, c35 C₆H₆ClNO: a148, c141 C₆H₆ClNO₂S: c42 C6H6Cl2N2: d215 C6H6Cl6: h26 C₆H₆FN: f9 C₆H₆HgO: p127 C₆H₆IN: i26 C₆H₆N₂O: e43, p250, p254 C₆H₆N₂O₂: n24, n25, n26 C₆H₆N₂O₃: a244, a245, m84

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₆H₆N₄O₄: d637 C₆H₆O: p64 C₆H₆OS: a57, m428 C₆H₆O₂: a44, d377, d378, d379, m251 C₆H₆O₂S: b20, t155 C₆H₆O₃: h146, m253, t304, t305 C₆H₆O₂S: b22 C₆H₆O₄: d460 C₆H₆O₅S: d382 C₆H₆O₆: p207 C₆H₆O₈S₂: d381 $C_6H_6S: t159$ C₆H₇AsO₃: b11 C₆H₇BO₂: b12 C₆H₇ClN₂: c202, c203, c204, c205 C₆H₇N: a298, a299, m398, m399, m400 C₆H₇NO: a257, a258, a259, m101, m403, p264, p265 C₆H₇NO₂S: b21 C₆H₇NO₃S: a118, a119, a120, s23 C₆H₇NO₆S₂: a117 C₆H₇NS: a293 C₆H₇N₃O: p258 $C_6H_7N_3O_2$: n67, n68, n69 C₆H₇O₂P: p135 C₆H₇O₃P: p136 C₆H₈AsNO₃: a115, a116 C₆H₈Cl₂O₂: h62, m221 C₆H₈N₂: a223, a224, a225, a226, a227, d238, m121, m257, p107, p108, p109, p118 C₆H₈N₂O: a208, o63 C₆H₈N₂O₂S: b25, s22 $C_6H_8N_2O_3S: d32$ C₆H₈N₄: p181 C_6H_8O : c331, d525, h40, m216 C₆H₈O₂: b375, c322, d364, h42, m214, v4

C₆H₈O₃: a36, d365, f43, h183 C₆H₈O₄: d524, d544 C₆H₈O₆: a312, g8, i59 $C_6H_8O_7$: c273 C₆H₀Br: b262 C₆H₉ClO: c78 C₆H₀ClO₃: e95, e96 C₆H₀F₂O₂: b484 C₆H₀NO: v11 C₆H_oNOS: m418 C₆H₉NO₂: b438 C₆H_oNO₆: n21 C₆H₉N₃: a158 C₆H₉N₃O₂: a159, c284, C₆H₁₀: c330, d488, h41, h82, m351 $C_6H_{10}N_2$: e172, p184 C₆H₁₀N₂O₂: c323 C₆H₁₀N₂O₄: d279 C₆H₁₀N₂O₅: a14 $C_6H_{10}N_4$: p26 C₆H₁₀O: c328, d26, d361, e5, e6, h78, m215, m350, m352 $C_6H_{10}O_2$: a96, c353, d359, e40, e104, e112, e166, h61, h71, h76, m349 C₆H₁₀O₃: d436, e53, e54, h121, p214 $C_6H_{10}O_4$: d325, d608, e17, h57, m272 $C_6H_{10}O_4S:t151$ C₆H₁₀O₄S₂: d709 C₆H₁₀O₅: d326 C₆H₁₀O₆: d616 $C_6H_{10}O_8$: t84 $C_6H_{10}S: d27$ C₆H₁₁Br: b261 $C_6H_{11}BrO_2$: b295, e76, e77, C₆H₁₁Cl: c77 C₆H₁₁ClO: h73 $C_6H_{11}ClO_2$: b433, c151,

C₆H₁₁Cl₃Si: c344 C₆H₁₁I: i32 C₆H₁₁N: d25, h63, m339, m416 C₆H₁₁NO: c329, e217, f35, m376, o57, t352 C₆H₁₁NO₂: e61 C₆H₁₂: c312, d498, d499, e84, h75, m213, m347, m348 C₆H₁₂Br₂: d86 C₆H₁₂ClN: c160 C₆H₁₂ClNO: c112 C₆H₁₂Cl₂: d187 C₆H₁₂Cl₂O: b161 C₆H₁₂Cl₂O₂: b156, d169 C₆H₁₂Cl₃O₃P: t417 C₆H₁₂Cl₃O₄P: t416 C₆H₁₂F₃NOSi: m440 C₆H₁₂NO₃P: d293a $C_6H_{12}N_2$: d45, t269 C₆H₁₂N₂O₃: s15 $C_6H_{12}N_2O_4S_2$: c371 C₆H₁₂N₂S₄: b174 C₆H₁₂N₂Si: t373 $C_6H_{12}N_4$: h52 $C_6H_{12}O$: a100, b488, c327, d497, d618, e87, h54, h72, h77, i72, m346, o47 $C_6H_{12}O_2$: b412, b413, b414, d500, e49, e88, e89, h66, h142, i62, m227, m302, m340, m341, m342, t77 $C_6H_{12}O_3$: d435, d457, d515, e37, e152, e154, i99, p2, p232, t67 $C_6H_{12}O_4Si: d23$ C₆H₁₂O₆: f36, g1, g6, i23, m11, s6 $C_6H_{12}O_7$: g4 $C_6H_{12}S: c326$ $C_6H_{13}Br: b294$ $C_6H_{13}BrO_2$: b267 C₆H₁₃Cl: c129 C₆H₁₃ClO: c130

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

C₆H₁₃ClO₂: c81 C₆H₁₃ClO₃: c105 C₆H₁₃Cl₃O₃Si: t415 C₆H₁₃I: i39 C₆H₁₃N: c334, h51, m371, m372, m373, m374 C₆H₁₂NO: d260, d553, e184, h144, p187 C₆H₁₃NO₂: a183, a184, h122, i79, L4, L5 C₆H₁₃NO₄: b182 C₆H₁₃NO₄S: m451 C₆H₁₃NO₅: g5, t428 C₆H₁₄: d489, d490, h55, m336, m337 C₆H₁₄ClN: d272 C6H14Cl4OSi2: b168 C₆H₁₄N₂: a182, a219, c318, c319 C₆H₁₄N₂O: a172, h123 C₆H₁₄N₂O₂: L12 C₆H₁₄N₄O₅: a311 C₆H₁₄O: b449, d417, d492, d492, d494, d495, d496, d701, e83, h68, h69, h70, m343, m344, m345 C₆H₁₄OSi: a97, e33, t374 $C_6H_{14}O_2$: b410, d251, d252, d491, e179, h58, h59, h60, i86, m338 C₆H₁₄O₂S: d704 C₆H₁₄O₃: b191, d253, e35, e156, h65, h172, t322 $C_6H_{14}O_4$: e127, t270 $C_6H_{14}O_4S: d703$ $C_6H_{14}O_6$: d738, m10, s5 $C_6H_{14}O_6S_2$: b188 C₆H₁₄S: b451, h64 C₆H₁₄Si: a104 C₆H₁₅Al: t263 C₆H₁₅As: t266 $C_6H_{15}B: t268$ C₆H₁₅Bi: t267 C₆H₁₅ClO₂Si: c154 C₆H₁₅ClO₃Si: c231 C₆H₁₅ClSi: b446

C6H15Ga: t274 C₆H₁₅In: t276 C₆H₁₅N: d411, d696, e85, e86, h80, m353a, t264 C₆H₁₅NO: a185, a216, a217, b419, b448, d270 C₆H₁₅NOSi: m439 C₆H₁₅NO₂: d254, e118 C₆H₁₅NO₃: t264 C₆H₁₅NO₆S: t424 C₆H₁₅N₃: a174 $C_6H_{15}O_3B$: t260 C₆H₁₅O₃P: d420, t282 C₆H₁₅O₃PS: t285 C₆H₁₅O₄P: t280 C₆H₁₅P: t281 C₆H₁₅Sb: t265 C₆H₁₆Cl₂Si₂: t104 C₆H₁₆N₂: d302, h56, t108 C₆H₁₆OSi: p218 C₆H₁₆Br₂OSi₂: b150 C₆H₁₆O₂Si: d249 C₆H₁₆O₃SSi: m22 C₆H₁₆O₃Si: t266b C₆H₁₆Si: t284 C₆H₁₇NO₃Si: a280 C₆H₁₇NO₅S: b180 C₆H₁₇N₃: i9 CaHaoLiNSia: L11 C₆H₁₈N₂Si: b172 C₆H₁₈N₃ClSi: c257a C₆H₁₈N₃OP: h53 C₆H₁₈N₄: t272 C₆H₁₈OSi₂: h50 C₆H₁₉O₂Si₂: h48 C₆H₁₉NOSi₂: b210 C₆H₁₉NSi₂: h49 C₆N₄: t37

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C₇F₅N: p23 C₇H₃BrClF₃: b250 C₇H₃BrF₃NO₃: b315

c184 Cl₂H₂ClN₂O₅: d630 C2H3ClN2O6: c96 C7H2Cl2O: d160, d161 C₇H₄BrF₃: b233, b234 C7H4ClFO: f14 C₇H₄ClF₃: c51, c52, c53 C₇H₄ClN: c47, c48 C7H4CINO: c206 C7H4ClNO3: n41, n42 C₇H₄ClNO₄: c178, c179, c180, n66 C₇H₄Cl₂O: c55, c56, d150 C₇H₄Cl₂O₂: d156, d157, d158 C7H4Cl3F: t233 C2H4Cl4S: t34 $C_7H_4F_3NO_2$: n88, n89 C7H4F12O: d718 C₇H₄I₂O₃: h111 $C_7H_4N_2O_3$: n40 C₇H₄N₂O₆: d628, d629 C7H4N2O7: d638 C7H4O3S: h104 C₇H₄O₄S: s24 C7H5BrO: b66, b228 C₇H₅BrO₂; b232 C7H5BrO2: b348 C₇H₅ClF₃N: a144, a145, a146 C7H5ClN2: a141 C₇H₅ClO: b67, c38, c39 C₇H₅ClOS: p103 C₇H₅ClO₂: c45, c46, c46a, c237, c238, p102 C₇H₅ClO₃: c193 C₇H₅Cl₂F: c119 C7H5Cl2N: d196 C₇H₅Cl₂NO: d151 C₇H₅Cl₃: t248, t249 C₇H₅FO: b69, f10 C₇H₅FO₅: f12, f13 $C_7H_5F_3$: t300

C₇H₅F₃N₂O₂: a241, a242

C₇H₅F₃O: t290

C₇H₃ClF₃NO₂: c182, c183,

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C7H5F4N: a179 C7H5IO2: i29 C7H5IO3: i51 C7H5I2NO2: a156 C₇H₅N: b51 C₇H₅NO: b63, p121 C₇H₅NO₃: n27, n28 C₇H₅NO₃S: s1 C₇H₅NO₄: n37, n38, n39, p259, p260, p261 C7H5NO5: h154 C₇H₅NS: b60, p122 C₇H₅NS₂: m17 C₇H₅N₃O₂: a238, n36, n55 C₇H₅N₃O₂S: a240 C7H5N3O6: t386 C7H6BrClO: b252 C₇H₆BrNO₂: n46 C7H6BrNO3: h155 C₇H₆Br₂: b236, d102 C₇H₆ClF: c123, c124, c125, f16 C₇H₆ClNO: c40 C₇H₆ClNO₂: a140, c187, c188, c189, n47 C₇H₆ClNO₃: c140 C₇H₆Cl₂: c59, c60, d229, d230, d231 C2H6Cl2O: d191, d192 C₇H₆F₃N: a129, a130, a131 C₇H₆INO₅: a203 C₇H₆N₂: a124, a125, a126, b38 C₇H₆N₂O₃: n29 C₇H₆N₂O₄: a237, d639, d640, d641 C₇H₆N₂O₅: d631, d33a C₇H₆N₂S: a128, m15 $C_7H_6O: b3$ C₇H₆OS: t143 C₇H₆O₂: b44, h94, h95, h96, m240 C₇H₆O₂S: m16 C₇H₆O₃: d375, d376, f41, h99, h100, h101

C₇H₆O₄: d383, d384, d385 C7H6O5: t306 C₇H₆O₆S: s28 C₇H₇Br: b85, b355, b356, b357 C₇H₇BrO: b235, b301, b302, b303 C₇H₇Cl: b89, c244, c245, c246 C₇H₇ClN₄O₅: c241 C₇H₇ClO: c57, c139, c158, c159 C7H7ClO2S: t177 C₇H₇ClO₃S: m49 C7H7CIS: c248 C₇H₇Cl₃Si: b123, t192 C₇H₇F: f24, f25, f26 C₇H₇FO: f15, f19 C₇H₇FO₂S: t178 C7H7I: i53, i54 C7H7IO: i41 C7H7N: v9, v10 C7H7NO: a53, a54, a55, b4, f31 $C_7H_7NO_2$: a121, a122, a123, h97, h98, m401, m402, n85, n86, n87 C₇H₇NO₃: a286, a287, m81, m82, m323, m324, n44, n45 C7H7NO4S: c16 C₇H₇N₃: a201, a202, m136 C₇H₈: b129, c310, t167 C7H8BrN: b304 C₇H₈ClN: c58, c142, c143, c144, c145, c146 C7H8CINO: c138a, c138 C₇H₈ClNO₂S: c247 C₇H₈Cl₂Si: d198, m358 C₇H₈N₂O: a114, b72, p165 $C_7H_8N_2O_7$: d33, h165, m315, m316, m317 C₇H₈N₂O₃: m78, m79, m80 $C_7H_8N_2S: p154$ C7H8N4O2: t138

C₇H₈O: b78, c279, c280, c281, m48 C₇H_oOS: m429 C₇H₈O₂: d389, d390, h105, m87, m88, m89, m276 C₇H₈O₂S: t173 C₇H₈O₃: e136, f45, m304 $C_7H_8O_3S: m127, t176$ C₇H_oS: m367, p128, t147 C₇H_oClSi: m357 C₇H₀N: b79, d604, d605, d606, d607, e211, e212, e213, m122, t180, t181, t182 C₇H₀NO: a218, b98, h126, m42, m43, m44 C7H0NO3: d456 C7H0NO2S: t174 C7H0NO3S: a294 C₇H₀NS: m422, m423 C₇H₀N₃O: a133 C_7H_{10} : b130 $C_7H_{10}N_2$: a157, a177, a178, d476, m360, t168, t169, t170, t171 $C_7H_{10}N_2O: m94$ C₇H₁₀N₂OS: h129 $C_7H_{10}N_2O_2$: e173, m232 $C_7H_{10}N_2O_2S$: a210, t175 $C_7H_{10}O: m61, m62, n108,$ t65 $C_7H_{10}O_2$: a40, c359 C₇H₁₀O₃: e12, h158, m333, t341 C7H10O4: d550 $C_7H_{10}O_5$: d459 C7H10Si: m366 $C_7H_{11}Br: b318$ $C_7H_{11}BrO_4$: d286 $C_7H_{11}ClO: c316$ $C_7H_{11}ClO_4$: d290 C₇H₁₁NO: c340, h110 C₃H₁₁NO₂: a52 C₇H₁₁NO₃: m335 C₇H₁₁NO₅: a45 C7H11NS: c341

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

C₇H₁₂: c311, h22, m207, m208, n107 C₇H₁₂O: c309, c315, m204, m205, m206, m268 $C_7H_{12}O_2$: b417, c317, d355, e121 C₇H₁₂O₃: e168, e195 $C_7H_{12}O_4$: d317, d318, d552, d574, d575, d576, h8, m273, t126 C₇H₁₂O₅: g17, g18 C₇H₁₂O₆Si: m435 C₇H₁₂O₇: g3 C₇H₁₃Br: b260, b306 C7H13BrO2: e80 C₇H₁₃ClO: h18 C₇H₁₃N: a250, d333, q5 C7H12NO: a317, c339 C₇H₁₃NO₂: a152 C₇H₁₄: c306, h19, m194 C₇H₁₄ClN: c113 C₇H₁₄N₂: d416 C₇H₁₄N₂O: a278 C7H14N2O2: e201 C₇H₁₄O: c308, c342, d569, d578, h5, h15, h16, h17, m197, m198, m199, m200, m201, m202, m203, m267 C₇H₁₄O₂: b479, c307, d258, e123, e170, e198, h10, i80, m75, m265, p52 C7H14O3: i68 C7H14O6: m256 C7H15Br: b291, b292 C7H15C1: c128 C7H15ClO2: c82 C7H15Cl3Si: h21 C7H15I: i37 C₇H₁₅N: c324, d591, e202, e203, m209, m211, m211 C₇H₁₅NO: d469, e157, h125, m375, p185, p186 C₇H₁₅NO₂: p276 $C_7H_{15}NO_3$: c18, m452 C7H15O5P: e119

C₇H₁₆: d570, d571, d572, d573, e197, h6, m264, t337 C₇H₁₆BrNO₅: a38 C7H16CINO3: a39 C₇H₁₆N₂: a215, m301, t366 C₇H₁₆N₂O: a277 $C_7H_{16}N_2O_2$: p182 C₇H₁₆O: d577, h12, h13, h14, m266, t338 C₇H₁₆O₂: d257, d331, m394 C₇H₁₆O₂Si: d256, e228 C₇H₁₆O₃: d700, t278, t321 C₇H₁₆O₄: t91 C7H16S: h9 C7H17N: h20, m269a C₇H₁₇NO: d275 C7H17NO2: b420, d274 C7H17NO5: m255 C7H17NO6S: t427 C₇H₁₇NO₇S: t426 C₇H₁₈N₂: d330, h7, i103, t118 C₇H₁₀N₂O: b173 C₇H₁₈N₂O₂: a276 C7H18O2Si: b486 C₇H₁₈O₃Si: b485, t266a C7H10NOSi2: b209 C₇H₁₉NSi: d343, t371 C₇H₁₀N₃: d42, t419 C₇H₂₁N₃Si: t420

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C₈Br₄O₃: t10 C₈Cl₄O₃: t31 C₈D₁₀: e67 C₈HCl₄NO₂: t32 C₈H₃NO₅: n72 C₈H₄BrNO₂: b296 C₈H₄Cl₂O₂: b14, b15, p171 C₈H₄Cl₆: b202 C₈H₄F₃N: t298 C₈H₄F₆: b206 C₈H₄N₂: d236, d237 C₈H₄O₃: p168 C₈H₅Br₅: p5 C₈H₅ClO₄: c209 C₈H₅Cl₃O₃: t242 C₈H₅F₃O: t289 C₈H₅F₃O₂S: t137 C₈H₅F₆N: b205 C_oH₅NO: b68 C₈H₅NO₂: i21, p170 C₈H₅NO₃: h166, i58 C₈H₅NO₆: n31, n32, n33, n34 C₈H₆: p82 C₈H₆BrClO: b246 C₈H₆BrN: b329 C₈H₆Br₂O: d64 C₈H₆Br₄: t11, t12 C₈H₆ClF₃: t299 CoHcClN: c201 C₈H₆ClNO₃: c171 C_oH_oCl_oO: d140 C₈H₆Cl₂O₃: d214 C_oH₆Cl₄: t35 C₈H₆N₂: q4 C₈H₆N₂O₂: a266, n65 C₈H₆N₂O₆: d636, m228 C₈H₆O: b42 $C_8H_6O_2$: b13, p169 C₈H₆O₃: b70, c14, f33, m239 $C_8H_6O_4$: b16, b17, m241, p167 C₈H₆S: b61 C₀H₇Br: b349 C₈H₇BrO: b221, b222 C₈H₇BrO₂: b327, b328 C₈H₇ClO: c28, c29, c30, p81, t187, t188, t189 CoH2ClOS: b91 C₈H₇ClO₂: b90, c200, m53, C₈H₇ClO₃: c86, c197, m184, m185 C₈H₇ClO₄: c133 C₈H₇FO: f8 C_8H_7N : i18, p80, t184, t185, t186

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₈H₇NO: m9, m137, t190 C₈H₇NO₂: h133, n84 C₈H₇NO₃: n22, n23 C₈H₇NO₃S: t179 C₈H₇NO₄: a116a, m318, m319, m320, m321, n62, n63, n64 C₈H₇NO₅: m83 C₈H₇NS: b121, m135 C₈H₇N₃O₂: a153 C₈H₈: s11 C₈H₈BrNO: b219 $C_8H_8Br_2$: d79, d104, d105 C₈H₈ClNO: c23 C₈H₈ClNO₃S: a10 C₈H₈Cl₂: d233, d234 C₈H₈Cl₂Si: p166 C₈H₈HgO₂: p125 C_oH_oN₂: a260, m128 C₈H₈N₂OS: a207 C_oH_oO: a31, e9, m126, p76a C₈H₈OS: m424, p153 C₈H₈O₂: b41, b97, h90, h91, h92, m45, m46, m129, m130, m131, m132, p78, p79 C₈H₈O₂S: t160 C₈H₈O₃: d370, d380, h130, h131, h137, h138, h160, m8, m50, m51, m52, m242, m277, m410, p68, t74 C₈H₈O₄: d21, h132 C₈H₈O₄S: a33 C₈H₉Br: b282, b283, b368, b369, b370, b371 C₈H₉BrO: b270, b286 C₈H₉BrO₂: b268 C₈H₉Cl: c107, c108, c258, c259, c260, c261 C₈H₉ClO: c90 C₈H₉N: b100, c360, i22, m447

C₈H₉NO: a18, a108, a109, a110, b96, m249 C₈H₉NO₂: a15, a16, a17, a211, a212, b88, d556, d557, d558, d559, e187, e214, e215, e216, m47, m116, m117, p115, t75 C₈H₀NO₃: a206, h163, h164, m85, n59 C₈H₀NO₄: d444 C₈H₁₀: e68, m244, x4, x5, x6 C₈H₁₀N₂O: d560 $C_8H_{10}N_4O_2$: c1, d240 C₈H₁₀O: b131, d579, d580, d581, d582, d583, d584, e28, e199, m105, m106, m107, m138, m139, m140, p112, p113 C₀H₁₀O₂: b18, d431, d432. d433, m54, p72, p111 C₈H₁₀O₃: c320, d446, h135, h159 C₈H₁₀O₃S: m434 C₈H₁₀O₄: d263 C₈H₁₀S: b105 C₈H₁₁ClSi: d585 C₈H₁₁N: b103, d477, d478, d479, d480, d481, d482, d483, e63, e64, e65, e180, e181, m141, m142, p114, t367 C₈H₁₁NO: a173, a256, a261, a262, a300, d470, e24, h117, m55, m71, m72, m73, p266 C₈H₁₁NO₂: d427, d428, d429 C₈H₁₁NO₂S: m433 C₈H₁₁NO₃: e132 C₈H₁₁NO₃S: d463 $C_8H_{11}N_5$: p93 C₈H₁₂: c345, v6 $C_8H_{12}N_2$: d239, d586, t119, x9 C₈H₁₂N₂O₂: d410 $C_8H_{12}N_2O_3$: d280 C₈H₁₂N₄: a323

C₈H₁₂O: e234 C₈H₁₂O₂: d508, e219, h185, n111 C₈H₁₂O₃: e194 C₈H₁₂O₄: d305, d316 C₈H₁₂O₆Si: t195 C₈H₁₂Si: d587 C₈H₁₃N: e235 C₈H₁₄: c349, d532, o17, o44, v5 C₈H₁₄N₂: p188 C₈H₁₄O: c348, d510, e7a, m262, o45 C₈H₁₄O₂: b459, c333, c363, d537, i69, m195 $C_8H_{14}O_3$: b415, b496, d712, e90 C₀H₁₄O₄: b447, d320. d335, d536a, e149, o24 C₈H₁₄O₄S: d619 $C_8H_{14}O_4S_2$: d708 $C_8H_{14}O_6$: d339, d340 C₈H₁₄O₆Si: t194 C₈H₁₅ClO: e145, o37 C₈H₁₅N: o27 C₈H₁₅NO: d367 C₈H₁₅NO₂: d468, e204, e205, e206 C₈H₁₆: c346, d506, d507, e108, o39, t357 C₈H₁₆ClN: c227 C₀H₁₆O: c347, d509, e109. e110, o34, o35, o36, o40 $C_8H_{16}O_2$: b431, c321, e142, e143, h79, i67, m261, o29, p234 C₈H₁₆O₄: e36, t125 C₈H₁₇Br: b320 C₈H₁₇Cl: c190 C₈H₁₇Cl₃Si: o43 C₈H₁₇I: i46 C₈H₁₇N: c350, d511 C₈H₁₇NO₂: p189 C₈H₁₇NO₃S: c335 $C_8H_{17}O_5P$: t283

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

C₈H₁₈: d533, e140, e174, e175, m260, o22, t100, t353, t354, t355 C₈H₁₈ClNO₅: a49 C₈H₁₈Cl₂O₂Si₃: d186 C₈H₁₈Cl₂Si: d184 C₈H₁₈Cl₂Sn: d136a C₈H₁₈F₃NOSi₂: b212 C₈H₁₈N₂: c314 C₈H₁₈N₂O: m224, m367 C₈H₁₈N₂O₄S: h124 C₈H₁₈O: d115, d407, e144, 030, 031, 032, 033 C₈H₁₈OSi₂: d713 C₈H₁₈OSn: d137 $C_8H_{18}O_2$: d122, d535, e141, o25, o26, t356 C₀H₁₀O₂S: d135 $C_8H_{18}O_3$: b176, b411, d698, t277 C₈H₁₈O₃S: d134 C₀H₁₀O₂Si: t262 C₈H₁₈O₄: b189 C₈H₁₈O₄S: d131 C₈H₁₈O₅: t51 C₈H₁₈S: d132, d133, o28 C₈H₁₈S₂: b153, b154, d113, d114 C₀H₁₀Si₂: b208 C₈H₁₉N: d107, d406, d418, d536, e147, o41, t102 C₈H₁₀NO: d412 C₈H₁₉NO₂: b444, d247, d248 C₈H₁₉NO₅: b183 $C_8H_{10}O_3P: d127$ C₈H₂₀BrN: t48 C₈H₂₀ClN: t49 C₈H₂₀Ge: t56 $C_8H_{20}N_2$: d534, o23, t101, t273 C₈H₂₀O₃SSi: m19 C₈H₂₀O₃Si: t261 C₈H₂₀O₄Si: t47

 $C_8H_{20}O_5P_2$: t59

 $C_8H_{20}O_7P_2$: t58

 $\begin{array}{l} C_8H_{20}Pb: t57 \\ C_8H_{20}Si: t60 \\ C_8H_{20}Sn: t62 \\ C_8H_{21}NO: t50 \\ C_8H_{21}NOSi_{2}: b207 \\ C_8H_{21}NO_2Si: a275 \\ C_8H_{22}N_2O_3Si: a167a, t324 \\ C_8H_{22}N_4: b145 \\ C_8H_{22}O_2Si_{2}: b211 \\ C_8H_{23}N_5: t54 \\ C_8H_{24}C_1O_3Si_4: d207 \\ C_8H_{24}O_2Si_3: o21 \\ C_8H_{24}O_4Si_4: o20 \\ C_8H_{28}N_4Si_4: o19 \end{array}$

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C₉F₁₅N₃: t432 C₀H₂Cl₆O₃: h30 C₉H₃Cl₃O₃: b32 $C_0H_4O_5$: b31, c15 C₀H₅BrClNO: b255 C₀H₅Br₂NO: d87 C₀H₅ClINO: c132 C₀H₅Cl₂N: d225 C₉H₆BrN: b347 C₀H₆ClN: c236 C₀H₆CINO: c134 C₀H₆N₂O₂: n77, t172 C₀H₆O₂: b56, c276 C₀H₆O₃: h108, h109 CoH6O4: i16 C₀H₆O₆: b28, b29, b30 C₀H₇BrO: b259 C₉H₇ClO: c268 C₀H₇ClO₂: c76 C₀H₇Cl₂O₂: t243 C₀H₇N: i110, q3 C₀H₇NO: h178, i20 C₀H₇NO₃: h143, m285 C₉H₇NO₄S: h179 C₉H₇N₃O₄S₂: a247 C₉H₈: i17 $C_0H_8Cl_2O_2$: n109 C₉H₈N₂: m409

C₉H₈N₂O₅: n43 C₀H₈O: c266, i15 C₀H₈O₂: c267, d353 C₀H₈O₃: h107 C₉H₈O₄: a56, p124 C_oH_oBrO: b342 C_oH_oCl: c217 CoHoClO: c223 C₀H₀ClO₃: c199, c249 CoHoN: d486, m283, m284 C_oH_oNO: m93 C₀H₀NO₂: a9 CoHoNOS: t191 C₀H₀NO₃: a11, a12, b71 C₀H₀N₃O: a265 C₉H₁₀: a84, i13, m411, v3 C₀H₁₀F₃NO₂: m123 C₉H₁₀N₂: a301, p119a C₀H₁₀N₂O: p147 $C_9H_{10}N_2O_2$: p83 C₀H₁₀N₂O₃: a132 C₀H₁₀O: a98, a99, c269, d360, i14, m113, p144, p145, p209, p217 $C_9H_{10}O_2$: b77, d485, e9a, e25, e26, e69, h170, h171, m39, m40, m41, m356, p74, p146 C₉H₁₀O₂S: b120 $C_9H_{10}O_3$: d430, e29, e30, e39, e48, e151, e218, m91, m279, m292, p75 C₉H₁₀O₄: d434, m288, m445 C₉H₁₀O₈: c354 C₉H₁₁Br: b297, b331, b361, b362 C₀H₁₁BrO: b343 C₉H₁₁ClO₃S: c114 C₀H₁₁Cl₃Si: c226, m354 C₉H₁₁N: a83, a199, a200, c332, t71, t80 C₉H₁₁NO: d462, m355, m432 C₉H₁₁NO₂: d464, e27, e59,

e60, p84

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₉H₁₁NO₃: t437 C₀H₁₂: e158, i91, n91, p222, t333, t334, t335, v8 C₉H₁₂Cl₂Si: m353 C₉H₁₂N₂O₄: a246 $C_0H_1,N_2O_6:u14$ C₀H₁₂O: b95, d547, d548, i106, i107, p142, p143, p235, t358, t359, t362 $C_0H_{12}O_2$: b110, e31, i85, n110, p73, p140, t348 $C_0H_{12}O_3$: m196, t315 C₀H₁₂O₃S: e222 $C_9H_{12}S: p141$ C₀H₁₃N: b480, d487, d622, e72, e169, e223, e224, i90, t330 C₉H₁₃NO: a264, b80, m86, n112 C₉H₁₃NO₂: a263 C₀H₁₃N₃O₂: t438 C₀H₁₄BrN: p159 C₀H₁₄Br₃N: p162 C₀H₁₄ClN: p160 C₀H₁₄IN: p161 $C_9H_{14}N_2$: n94 C₀H₁₄O: d527, d529, i82, t340 C₀H₁₄OSi: t375 C₉H₁₄O₂Si: d443 C₉H₁₄O₃: b192 C₉H₁₄O₃Si: p158 C₀H₁₄O₅: d262, d321 $C_9H_{14}O_6$: p201 C₉H₁₄Si: p163 C₉H₁₅NO: c361 C₀H₁₅NO₂: d568 C₉H₁₅NO₅: d261 C₀H₁₅NSi: t369 C₉H₁₆: h46 C₉H₁₆Cl₂Si: c333a C₉H₁₆N₂: d46 C₉H₁₆O: d528 C₉H₁₆O₂: c325 C₉H₁₆O₃: b467

C₀H₁₆O₄: d303, d307, d322, d530, n95 C₀H₁₇ClO: n101 CoH17N: a88, n97 C₉H₁₇NO: m180 C₀H₁₇NO₂: e177, e178 C₉H₁₈: i94, n102, p224, t339 C₉H₁₈NO: t117 C₉H₁₈N₂O₃Si: t325 C₀H₁₈O: d531, n100, n103 C₉H₁₈O₂: e138, m329, n98 C9H18O3: d111 C₀H₁₀Br: b317 C₉H₁₉N: i95, t332 C₉H₁₉NO: d116 C₉H₁₉NO₂: e120 C₉H₁₉NO₃S: c337 C₉H₂₀: n92, t346 C₀H₂₀Cl₂Si: m330 C₉H₂₀N₂: a296 C₀H₂₀N₂S: d136 C₉H₂₀O: n99, t347 C₉H₂₀O₂: b450, n96 C₉H₂₀O₃: d699, t279 C₉H₂₀O₃Si: a103 CoH20O4: t408 C₉H₂₀O₅: t53 C₀H₂₁BO₃: t406 C₉H₂₁ClO₃Si: c230 C₀H₂₁ClSi: c257 C₉H₂₁N: n104, t407 C₀H₂₁NO₃: t309 C₀H₂₁N₃: t275 C₉H₂₁O₃B: t310 $C_0H_{21}O_3P: t313$ C₀H₂₂N₂: d327, n93 C₀H₂₂O₃Si: p238 C₉H₂₃NO₃Si: a279 C₉H₂₄N₄: b147

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C₁₀H₂O₆: b27 C₁₀H₄Cl₂O₂: d201

C₁₀H₆N₂: b99 C₁₀H₆N₂O₄: d634 $C_{10}H_6N_2O_4S: d48$ C₁₀H₆O₂: n11 C₁₀H₆O₃: h152 C₁₀H₆O₈: b26 $C_{10}H_7Br: b312$ $C_{10}H_7BrO: b313$ C₁₀H₇Cl: c168, c169 C₁₀H₇NO₂: n57, n81, p123 C₁₀H₇NO₈S₂: n82 C₁₀H₈: a326, n2 C₁₀H₈BrNO₂: b287 C₁₀H₈N₂: d705 $C_{10}H_8O: n9, n10$ C₁₀H₈O₂: d392, d393, d394, d395, m191 C10H8O3: h140 C₁₀H₈O₃S: n18 C₁₀H₈O₇S₂: h150, h151 C10H8O8S2: d396 $C_{10}H_0ClCrN_2O_3$: b143 $C_{10}H_0N$: m407, m408, n17 $C_{10}H_0NO$: a51, a236 C₁₀H₀NO₂: i19 C₁₀H₉NO₃S: a234 C₁₀H₉NO₄S: a193, a194, a195, a196 $C_{10}H_9NO_6$: d561 $C_{10}H_9NO_6S_2$: a232, a233 $C_{10}H_9N_3$: d706 $C_{10}H_{10}CIFO$: c120 $C_{10}H_{10}CINO_2$: c26 $C_{10}H_{10}N_2$: a285, n4, n5 $C_{10}H_{10}N_2O: m365$ $C_{10}H_{10}O: d362, m190, p96,$ p98 $C_{10}H_{10}O_2$: b64, s2 $C_{10}H_{10}O_3$: b73, m60 $C_{10}H_{10}O_4$: d588, d589, d590, h136, p152 $C_{10}H_{11}BrO: b312a$ $C_{10}H_{11}ClO_3$: c198 C₁₀H₁₁ClO₄: t317 C₁₀H₁₁IO₄: i28

C₁₀H₁₁N: p101

TABLE 1.14 Empirical Formula Index for Organic Compounds (continued)

C₁₀H₁₁NO₂: a32, d448 C10H11NO4: c10 C₁₀H₁₁NO₆: m226 C₁₀H₁₂: d244, t73 C10H12NO: b408 $C_{10}H_{12}N_2$: a170, b81, b102 $C_{10}H_{12}N_2O_2$: p77 C₁₀H₁₂O: a94, b500, e55, i77, m97, m386, m387, m391, p94, p95 $C_{10}H_{12}O_2$: e200, h112, h162, m70, m92, m98, m99, m100, p99, p100, p223 $C_{10}H_{12}O_3$: d426, e41, e163, m300, p71, p230 $C_{10}H_{12}O_4$: d447, m225, t314 $C_{10}H_{12}O_5$: d306, p239, t316 C10H12O6: d514 C₁₀H₁₃Br: b298 C₁₀H₁₃BrO: b243 C₁₀H₁₃Cl: b434 C₁₀H₁₃NO: p129 C₁₀H₁₃NO₂: e45 C₁₀H₁₃NO₂S: b92 C10H13N5O4: a70 C₁₀H₁₄: b423, b424, b425, d282, d283, d284, i64, i100, i101, i102, t97, t98, t99 $C_{10}H_{14}NO_5PS: p3$ C₁₀H₁₄N₂: n20, p139 $C_{10}H_{14}N_2O$: d323, d334 C₁₀H₁₄N₄O₄: d399 C10H14N5O7P: a72 $C_{10}H_{14}O$: b469, b470, b471, b472, b473, b477, c20, c362, i92, i102a, p58, t116, t254 C₁₀H₁₄O₂: b432, b454, d450 C₁₀H₁₄O₃: c6, c9 C₁₀H₁₄O₄: m90, t318 C₁₀H₁₅BrO: b245

C₁₀H₁₅N: b421, d277, d278, d564, e233, i93, p97, t96 C₁₀H₁₅NO: d273, e1, e2 C₁₀H₁₅NO₂: d451, p106 C10H15N5O10P2: a71 C₁₀H₁₆: a67, c2, d649, L6, L7, m453, p25, p175, p176, t5, t6, t253 C10H16CIN: b126 C10H16Cl2O2: d11 C₁₀H₁₆N₂O₈: e125 C₁₀H₁₆O: c3, c4, d352, d562, d563, L8, p177, p178, p243, t351 C10H16OSi: d519 C₁₀H₁₆O₄: c5, d266 C10H16O4S: c7 C₁₀H₁₆O₅: d265, d301 C10H16Si: b127 C₁₀H₁₇N: a66, p274 C₁₀H₁₇NO: c343, m450 $C_{10}H_{18}$: d1, d2, p174 C10H18N2O7: h119 C₁₀H₁₈O: b216, b441, b442, c265, d3, g2, i60, i83, i109, L9, m13, p190, t7, t350 C10H18O2: e112 $C_{10}H_{18}O_3$: d599, t70 $C_{10}H_{18}O_4$: b175, d9, d121, d332, d565 C10H18O4S: d341 C₁₀H₁₈O₆: d421 C10H19ClO: d17 C₁₀H₁₉N: d12, t331 C₁₀H₁₉NO₂: e207 C₁₀H₂₀: c301, d18 $C_{10}H_{20}Br_2$: d73 C₁₀H₂₀N₂S₄: t61 C₁₀H₂₀O: b439, b440, c274, d6, d16, d357, d366, e148, m12, m303 C₁₀H₂₀O₂: d14, e146, e190, m63, m170 C₁₀H₂₀O₅: p45

C10H20O5Si: t326 C10H21Br: b265 C10H21Cl: c80 C10H21I: i33 C10H21N: d294 C10H21NO: a230 C10H22: d7 C10H22N2: d41 C₁₀H₂₂O: d15, d651, t72 C10H22O2: d10, d106 C₁₀H₂₂O₃: d697, t413 C10H22O3S: d13 C₁₀H₂₂O₄: t412 C10H22O5: b190 C10H22O7: d648 C₁₀H₂₃N: d19, d650 C₁₀H₂₃NO: d108 C₁₀H₂₃NO₂: d259 $C_{10}H_{24}N_2$: d8, t55, t111 C₁₀H₂₄N₂O₂: d645 C10H24N4: b146 $C_{10}H_{24}OSi: m109$ C10H24O3Si: m441 C10H24O6Si: t429 C₁₀H₂₇O₃N₃Si: t323 C10H30O3Si4: d5 C10H30O5Si5: d4

C_{11}

C11H4F20O: i1 C₁₁H₇N: c293 $C_{11}H_8O: n1$ C₁₁H₈O₂: h147, m310, n3 $C_{11}H_8O_3$: h148, h149 C₁₁H₉Br: b309 C₁₁H₀Cl: c157 $C_{11}H_0N: p148$ C₁₁H₁₀: m308, m309 $C_{11}H_{10}N_2S: n19$ C₁₁H₁₀O: m76, m77 C₁₁H₁₁N: n6 C₁₁H₁₂N₂O: a309 C₁₁H₁₂N₂O₂: t436 $C_{11}H_{12}O_2$: d358, e103, m104

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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₁₁H₁₂O₃: e70 C₁₁H₁₃ClO: b428 C₁₁H₁₃ClO₃: c250 C₁₁H₁₃NO: b119 C₁₁H₁₃NO₂: t183 C₁₁H₁₃NO₃: a302, a303 C₁₁H₁₃N₃O: a113 C₁₁H₁₃N₃O₃S: d567 $C_{11}H_{14}O: m103, p43$ C₁₁H₁₄O₂: b426, b427, d455, e46 C₁₁H₁₄O₃: b409, b468, b476, e167 C₁₁H₁₄O₄: e155 C₁₁H₁₄O₄Si: d24 C11H15NO: d269 C₁₁H₁₅NO₂: d276, d466, C₁₁H₁₆: b482, p24, p54 C₁₁H₁₆N₂: b114 C₁₁H₁₆O: b86, b461, b462, p56 $C_{11}H_{16}O_2$: a68 $C_{11}H_{16}O_3$: m299 $C_{11}H_{16}O_4$: d714 $C_{11}H_{17}N$: b429, e160 C₁₁H₁₇NO: e225 C₁₁H₁₇NO₂: b104 C₁₁H₁₇O₃P: b93 $C_{11}H_{18}O: d308, n105, p4$ C11H18O5: d264 C₁₁H₁₉ClO: u11 C₁₁H₁₉N: a209 C₁₁H₂₀O: p55, u7 C₁₁H₂₀O₂: u9 C₁₁H₂₀O₄: d119, d287, d309 C₁₁H₂₁BrO₂: b367 C11H22: u8 $C_{11}H_{22}N_2$: d695 C₁₁H₂₂O: u1, u5, u6, u10 C₁₁H₂₂O₂: m218, u3 C11H22O4Si: e7 C₁₁H₂₃NO₂: a297 C₁₁H₂₄: u2 C₁₁H₂₄O: d310, u4 C₁₁H₂₄O₃Si: t311

C₁₁H₂₄O₄: t410 C₁₁H₂₄O₆: p46 C₁₁H₂₄O₆Si: t430 C₁₁H₂₆N₂: d129 C₁₁H₂₆N₂O₆: b214

C_{12}

C₁₂Br₁₀O: b197 $C_{12}H_4Cl_6S_2$: b203 C₁₂H₅ClO₃: c170 C12H6Br4O4S: s25 C₁₂H₆O₃: n7 C₁₂H₆O₁₂: b19 C₁₂H₇NO₂: n8 C₁₂H₈: a3 C₁₂H₈Br₂: d66 C12H8Cl2OS: b166 C₁₂H₈Cl₂O₂S: b165 $C_{12}H_8N_2$: p63 C₁₂H₈N₂O₂: a235 C₁₂H₈N₂O₄S₂: b194, b195 C₁₂H₈O: d50 $C_{12}H_8O_6$: b132 C12H8S: d52 $C_{12}H_9Br: b237$ C₁₂H₉BrO: b330 C₁₂H₉ClO₂S: c207 C₁₂H₉N: c8, d665, n16 $C_{12}H_9NO: b74, b75, b76$ C₁₂H₀NO₂: n48, n49 C₁₂H₉NO₃: n70, n71 C₁₂H₉NS: p66 $C_{12}H_{10}$: a2, b134 C₁₂H₁₀ClN: c61, c62 C₁₂H₁₀ClO₃P: d662 C₁₂H₁₀ClP: c99 C₁₂H₁₀Cl₂Si: d175 C₁₂H₁₀Hg: d675 C₁₂H₁₀N₂: a322 C₁₂H₁₀N₂O: n80, p89 C₁₂H₁₀N₂O₂: n52 C₁₂H₁₀N₂O₂S: a243 C₁₂H₁₀N₃O₃P: d682

 $C_{12}H_{10}O: d667, m311,$ m312, p131, p132 C₁₂H₁₀OS: d690 $C_{12}H_{10}O_2$: d387, h88, n14, $C_{12}H_{10}O_2S$: d689, t150 $C_{12}H_{10}O_3$: n12 C₁₂H₁₀O₃S: b139 $C_{12}H_{10}O_4$: q1 $C_{12}H_{10}O_4S$: s27, t145 $C_{12}H_{10}S$: d688 C12H10S2: d664 C₁₂H₁₀Se₂: d663 C₁₂H₁₁ClNO₂P: p134 $C_{12}H_{11}N$: a134, a135, b117, b118, d655 $C_{12}H_{11}NO: n13, p70$ $C_{12}H_{11}N_3$: p87 $C_{12}H_{11}O_3P: d681$ C₁₂H₁₂: d554, d555 $C_{12}H_{12}N_2$: b136, d673, p131 C₁₂H₁₂N₂O: o62 C₁₂H₁₂N₂O₂: b40 $C_{12}H_{12}N_2O_2S$: d36, d37 $C_{12}H_{12}N_4$: d31 $C_{12}H_{12}O: e44$ C₁₂H₁₂O₂Si: d687 C₁₂H₁₂O₃: t196 $C_{12}H_{12}O_6$: t193, t336 $C_{12}H_{13}N_3$: d34 C12H14N2O3S: a167 $C_{12}H_{14}N_4O_2S: s21$ $C_{12}H_{14}O_3$: e176 C₁₂H₁₄O₄: d329 C₁₂H₁₅N: d369 C₁₂H₁₅NO: b116 C₁₂H₁₅N₃O₃: t197 C₁₂H₁₆: c338, m212, p104 C₁₂H₁₆O₂: m364 C₁₂H₁₆O₃: d246 $C_{12}H_{17}N: b115, c337$ $C_{12}H_{17}NO: d319, d342$ C₁₂H₁₈: b489, c304, d414, d415, h47, p117, t435

C₁₂H₁₈Cl₂N₄OS: t139

TABLE 1.14 Empirical Formula Index for Organic Compounds (continued)

C₁₂H₁₈O: d419, d513 C₁₂H₁₈O₂: b474, b475 C₁₂H₁₈O₄: b445 C₁₂H₁₀N: d413, h81 C₁₂H₂₀O₂: b185, b217, e102, L10 C₁₂H₂₀O₃Si: p157 C12H20O4: d118 C12H20O4Si: t8 C12H21N: t431 C12H21N3: t422 C₁₂H₂₂: c305, d241 C12H22O: c303, e4 C12H22O3: h67 C₁₂H₂₂O₄: d130, d324, d512, d702, d721 $C_{12}H_{22}O_{11}$: L3, m7, s20 C12H22ClO: d728 C₁₂H₂₃N: d242, d724 C₁₂H₂₃NO: a318 C₁₂H₂₄: d729 C12H24N2: d694 C₁₂H₂₄O: c302, d731, m443, t349 C₁₂H₂₄O₂: d726, e113 C₁₂H₂₄O₆: h74 C₁₂H₂₅Br: b275 C₁₂H₂₅Cl: c100 C₁₂H₂₅Cl₃Si: d736 $C_{12}H_{26}$: d719 C₁₂H₂₆O: d350, d727, t354a C₁₂H₂₆O₂: d722, d723 C₁₂H₂₆O₃: b151 $C_{12}H_{26}O_4$: t411 $C_{12}H_{26}O_4S$: d735 $C_{12}H_{26}S: d725$ C₁₂H₂₇Al: t307 C₁₂H₂₇BO₃: t209 C₁₂H₂₇ClSn: t215 C₁₂H₂₇N: d349, d732, t210 C₁₂H₂₇O₃P: t214 C₁₂H₂₇O₄P: t212 C₁₂H₂₇P: t213 C₁₂H₂₈BrN: t135 C₁₂H₂₈N₂: d720

 $\begin{array}{l} C_{12}H_{28}O_4Si:t88,t134\\ C_{12}H_{28}O_4Ti:t166\\ C_{12}H_{28}O_8Si:t89\\ C_{12}H_{36}O_4Si_4Ti:t90 \end{array}$

C_{13}

C13H5N3O7: t384 C13H8CINO3: c181 C₁₃H₈ClNOS: p67 C₁₃H₈Cl₂O: d159 C13H8N2O2: b193 C₁₃H₈O: f3 C₁₃H₈OS: t165 $C_{13}H_8O_2$: x3 C₁₃H₉BrO: b232 $C_{13}H_{0}ClO: c49, c50$ C13H0ClO2: c131 C13H0N: a61 C13H10: f2 C₁₃H₁₀ClNO: a142, a143, d659 C₁₃H₁₀Cl₂O₂: m233 C₁₃H₁₀N₂: p90 C13H10N2O3: a239 $C_{13}H_{10}O: b53, x1$ C₁₃H₁₀O₂: b135, h102, p91 $C_{13}H_{10}O_3$: d386, d661, p150 $C_{13}H_{10}O_5$: t83 C₁₃H₁₁Br: b274 C13H11Cl: c97 C13H11ClO: c44 C13H11NO: a127, b5 C₁₃H₁₁NO₂: h161, p85 C13H11NO3: p86 C13H12: d676 $C_{13}H_{12}N_2$: b54, d38, d670 C₁₃H₁₂N₂O: d693 $C_{13}H_{12}N_2S$: d692, t146 C₁₃H₁₂N₄O: p88 C13H12N4S: d691 C₁₃H₁₂O: b138, d677, h113, m56, p76 $C_{13}H_{12}S: b113$

C13H13ClSi: c98 C₁₃H₁₃N: d678, m230, m93 C₁₃H₁₃NO: b106 C13H13N3: d671 $C_{13}H_{14}N_2$: d35, m238, t344 C13H14N2O3: a59 C₁₃H₁₄N₄O: d660 C₁₃H₁₄Si: m231 $C_{13}H_{16}O_{2}$: m74 C13H16O3: e71 C13H16O4: d328 C13H17NO2: e74 C₁₃H₂₀: p116 C13H20N2O2: d271 C13H20O: i56, i57 C13H22CIN: b125 C₁₃H₂₂N₂: d243 $C_{13}H_{22}O_{2}$: n106 C13H22O3Si: b124 C13H26: t258 C₁₃H₂₆N₂: m236, t343 C₁₃H₂₆O₂: e229, t257 C₁₃H₂₇Br: b359 C13H28: t256 C13H28O4: t409 C13H29NO4: b169

C_{14}

C₁₄H₆Cl₂O₂: d148, d149 C₁₄H₇ClO₂: c36, c37 C₁₄H₈ClNO₅: c185 C₁₄H₈O₂: a305, p62 C₁₄H₈O₃: h93 C₁₄H₈O₄: d371, d372, d373, d374 C₁₄H₈O₅S: a308 C₁₄H₈O₈: a306, d312 C₁₄H₉Si: b324 C₁₄H₉ClO₃: c54 C₁₄H₉ClO₃: c54 C₁₄H₉NO₂: a111, a112 C₁₄H₉NO₃: a186 1.78 SECTION 1

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

C₁₄H₁₀: a304, d654, p61 C₁₄H₁₀Br₂O: b273 C14H10ClNO3: a147 C₁₄H₁₀Cl₂O₄: b162 C14H10Cl4: b163 C₁₄H₁₀N₂O₂: d28, d29, d30 $C_{14}H_{10}O_2$: b34 C₁₄H₁₀O₃: b45, b65, x2 C₁₄H₁₀O₄: b137, d54, t82 C₁₄H₁₁N: d653, p120 C₁₄H₁₁NOS: a50 $C_{14}H_{12}$: d351, s9 C14H12Cl2O: b164 C₁₄H₁₂N₂O: b37 C₁₄H₁₂N₂O₂: b35 C₁₄H₁₂O: a34, d22, m133, m134 C₁₄H₁₂O₂: b46, b83, b84, b107, b108, d652 C₁₄H₁₂O₃: b36, h35 C14H13ClO: c147 C₁₄H₁₃N: e93, i12 C₁₄H₁₃NO: b82 C₁₄H₁₃NO₂: b50 C14H14: d666 C14H14N2: a168 C₁₄H₁₄N₂O₃: a325 C14H14O: d58 C₁₄H₁₄OS: b200 C₁₄H₁₄O₂: b109 C₁₄H₁₄S₂: b199, d57 C₁₄H₁₅N: d56, d668 C₁₄H₁₅O₃P: d61 C₁₄H₁₆N₂: d669 C₁₄H₁₆O₂Si: d437 C₁₄H₁₆O₄: d281 C14H18O4: d285 $C_{14}H_{20}N_2O_6S: m120$ $C_{14}H_{20}O_5$: b39 C₁₄H₂₂: p130a $C_{14}H_{22}O: d123, d124,$ d125, d126 $C_{14}H_{22}O_2$: d112 C₁₄H₂₃N: d109, o42 $C_{14}H_{23}N_3O_{10}$: d299 C14H26O3: h11 C14H26O4: d408

 $\begin{array}{l} C_{14}H_{27}CIO:t41 \\ C_{14}H_{28}:t42,t43 \\ C_{14}H_{28}O_{2}:t39 \\ C_{14}H_{29}Br:b352 \\ C_{14}H_{29}Cl_{3}Si:t46 \\ C_{14}H_{30}:t38 \\ C_{14}H_{30}O:t40 \\ C_{14}H_{31}N:t44 \\ C_{14}H_{32}N_{2}O_{4}:t87 \end{array}$

C_{15}

C₁₅H₁₀O₂: b101, m124 C₁₅H₁₁NO: d679 C₁₅H₁₂N₂O₂: d672 C₁₅H₁₂O: d354, d685 C15H12O2: d53 C₁₅H₁₃NO: a13 C15H14O: d684 C₁₅H₁₄O₅: b49, b141, d686 C15H14O3: b111 C₁₅H₁₆O: m359 C15H16O2: i97 C15H17N3: d711 C₁₅H₁₈OSi: e42 C₁₅H₂₂O₃: d117 C₁₅H₂₄: t312 C₁₅H₂₄O: d120 C₁₅H₂₆O: h184 C15H26O6: g19 C₁₅H₃₀N₂: t342 C₁₅H₃₀N₃OP: t405 C₁₅H₃₀O: p14 C₁₅H₃₀O₂: m413 $C_{15}H_{32}$: p13 C₁₅H₃₂O₃Si₄: p164 C₁₅H₃₂O₁₀: t389

 C_{16}

C₁₆H₁₀: b52, fl, p246 C₁₆H₁₁NO₂: p149 C₁₆H₁₂N₂O₅S: a60 C₁₆H₁₂N₄O₉S,: t3

C₁₆H₁₃N: p130 C₁₆H₁₄: d656, d657, e66 C₁₆H₁₄O: d658 C₁₆H₁₄O₆S: s26 C₁₆H₁₅NO₄: d445 C₁₆H₁₆O₂: b47, b112 C₁₆H₁₆O₃: d449 C₁₆H₁₈ClN₃S: m237 C₁₆H₁₉ClSi: b435 $C_{16}H_{20}N_2$: d59 C₁₆H₂₀O₂Si: d250 C₁₆H₂₂O₄: d128, d409 C₁₆H₂₂O₁₁: g7 C₁₆H₂₆O₃: d730 C₁₆H₂₆O₇: t52 C₁₆H₃₂: h37 C₁₆H₃₂O₂: h35 C₁₆H₃₃Br: b293 C₁₆H₃₃I: i38 C₁₆H₃₃NO: d297 C₁₆H₃₄: h4, h32 C₁₆H₃₄O: h36 $C_{16}H_{34}O_{2}$: h33 C₁₆H₃₄S: d644, h34 C₁₆H₃₅N: d643, h38 C₁₆H₃₅O₄P: b178 C₁₆H₃₆BF₄N: t19 C₁₆H₃₆BrN: t14 C₁₆H₃₆ClN: t15 C₁₆H₃₆FN: t16 $C_{16}H_{36}IN: t18$ $C_{16}H_{36}O_4Si: t13$ $C_{16}H_{36}Sn: t20$ C₁₆H₃₇NO₄S: t17

C_{17}

 $C_{17}H_6O_7$: b55 $C_{17}H_{10}O$: b8 $C_{17}H_{12}O_3$: p119 $C_{17}H_{13}N_3O_5S_2$: p172 $C_{17}H_{16}O_4$: d60 $C_{17}H_{18}O_3$: b478 $C_{17}H_{20}N_2O$: b171 $C_{17}H_{20}N_4O_6$: r4

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

$$\begin{split} &C_{17}H_{21}NO_4{:}c275\\ &C_{17}H_{22}N_2{:}m234\\ &C_{17}H_{23}NO_3{:}a315\\ &C_{17}H_{34}O_2{:}m263\\ &C_{17}H_{36}{:}h1\\ &C_{17}H_{37}N{:}m229 \end{split}$$

 C_{18}

C₁₀H₀Cl₆O₄P: t418 C₁₈H₁₀O₆: h85 C₁₈H₁₂: b6, b7, t396 C18H12N5O6: d683 C18H14: t4 C18H14O: d680 C₁₈H₁₄O₈: d55 C₁₈H₁₅As: t394 C₁₈H₁₅N: t392 C₁₈H₁₅N₃Si: a320 C₁₈H₁₅O₃P: t403 C₁₈H₁₅O₄P: t399 C18H15P: t400 C₁₈H₁₅PS: t402 C₁₈H₁₅PSe: t401 C₁₈H₁₅Sb: t393 C₁₈H₁₆O₂: b422 C₁₈H₁₆Si: t404 C18H18O3: e73 C₁₈H₂₀O₂: b48 C18H25NO3: i61 C₁₈H₃₀O: t211 C18H30O2: 07 C₁₈H₃₁N: d733 C18H32O2: 01 C₁₈H₃₂O₁₆: r1 $C_{18}H_{34}O_2$: o10, o11 C₁₈H₃₄O₄: d110 $C_{18}H_{36}$: d734, o8 C₁₈H₃₆O: o12 $C_{10}H_{26}O_{2}$: e139, o5 C₁₈H₃₇Br: b319 C₁₈H₃₇Cl₃Si: o15 C₁₈H₃₇N: o9 C18H37NO: 02

C18H38: 03

C₁₈H₃₈O: o6

C₁₈H₃₈S: 04 C₁₈H₃₉ClSi: t302 C₁₈H₃₉N: 013, t301 C₁₈H₃₉O₇P: t414 C₁₈H₄₀Si: t303

 C_{19}

C10H15Br: b366 C19H15Cl: c256 C₁₉H₁₆: t397 C19H16O: t398 C₁₉H₁₈BrP: m442 C₁₉H₂₀Br₄O₄: i96 C₁₉H₂₀O₄: b87 C₁₉H₂₂N₂O: c264 C₁₀H₃₀O₅: m243 $C_{19}H_{32}$: p156 C₁₀H₃₄ClN: b122 C₁₉H₃₄O₂: m325 C₁₉H₃₆O₂: m327 C₁₉H₃₇NO: o14 C₁₉H₃₈O₂: m326 C₁₉H₄₀: n90, t115 C₁₉H₄₀Cl₂Si: m328

 C_{20}

C20H10Br2O5: d83 C₂₀H₁₂: b57, b58, d49 C20H12O5: f4 $C_{20}H_{14}O_4$: p65 C₂₀H₁₅Br: b365 C₂₀H₁₈O₃Si: t391 C20H19N3: b2 C20H22O6: t271 $C_{20}H_{24}N_2O_2$: q2 C20H24O6: d51 C20H28O2P: d674 C20H30O2: a1 C20H31N: d20 C₂₀H₃₅N: t45 C20H36O2: e188 C₂₀H₃₈O₂: e189 C20H40: i3

C₂₀H₄₀O: o16 C₂₀H₄₂: i2

 C_{21}

$$\begin{split} &C_{21}H_{15}NO: b142\\ &C_{21}H_{15}N_3O_3: t390\\ &C_{21}H_{21}N: t200\\ &C_{21}H_{22}N_2O_2: s10\\ &C_{21}H_{24}O_2: b144\\ &C_{21}H_{28}N_2O: b170\\ &C_{21}H_{36}O: p15\\ &C_{21}H_{30}N_3: t255 \end{split}$$

 C_{22}

 $\begin{array}{c} C_{22}H_{23}N_3O_9; \ a316 \\ C_{22}H_{30}O_2S; \ t144 \\ C_{22}H_{34}O_4; \ b443 \\ C_{22}H_{39}N; \ h39 \\ C_{22}H_{42}O_4; \ d312 \\ C_{22}H_{44}O_2; \ b466, \ d716 \\ C_{22}H_{46}; \ d715 \\ C_{22}H_{46}0; \ d717 \end{array}$

 C_{23}

C₂₃H₁₆O₆: m235 C₂₃H₂₆N₂O₄: b372

 C_{24}

 $\begin{array}{l} C_{24}H_{16}N_2O_2 \cdot b198 \\ C_{24}H_{18} \cdot t395 \\ C_{24}H_{20}BNa: t128 \\ C_{24}H_{20}O_4Si: t127 \\ C_{24}H_{20}Si: t132 \\ C_{24}H_{20}Si: t133 \\ C_{24}H_{20}Sn: t133 \\ C_{24}H_{22}N_2O: b140 \\ C_{24}H_{38}O_4 \cdot b179, d313 \\ C_{24}H_{40}O_5 \cdot c263 \\ C_{24}H_{40}O_5 \cdot c263 \\ C_{24}H_{50} \cdot t36 \\ C_{24}H_{50} \cdot t36 \\ C_{24}H_{50} \cdot t36 \\ C_{24}H_{51}N \cdot t387 \\ \end{array}$

TABLE 1.14 Empirical Formula Index for Organic Compounds (continued)

C ₂₄ H ₅₁ O ₃ P: d423, t421 C ₂₄ H ₅₂ O ₄ Si: t85 C ₂₄ H ₅₄ OSn ₂ : b201	C ₂₇ H ₄₆ O: c262 C ₂₇ H ₅₀ ClN: b94	C ₃₂ H ₆₈ O ₄ Si: t86 C ₃₆ H ₇₅ O ₃ P: d642 C ₃₈ H ₃₀ NiO ₂ P ₂ : b213 C ₃₀ H ₇₄ O ₆ : g20
C ₂₆	C ₂₈ C ₂₈ H ₂₇ : t129	C ₃₀ H ₇₄ O ₆ , g20 C ₄₀ H ₅₆ : c19 C ₄₀ H ₈₂ O ₆ P ₂ : b196
C ₂₆ H ₂₀ : t131 C ₂₆ H ₂₆ N ₂ O ₂ S: b152	C ₂₈ H ₃₂ C ₁ Si ₃ : r2 C ₂₈ H ₃₂ O ₂ Si ₃ : t121	C ₄₅ to C ₅₇
C ₂₆ H ₂₆ OSi ₂ : t130 C ₂₆ H ₅₀ O ₄ : b177, d311	C ₃₀ to C ₄₀	C ₄₅ H ₈₆ O ₆ : g24 C ₄₈ H ₄₀ O ₄ Si ₄ : o38
	$C_{30}H_{50}$: s8 $C_{30}H_{62}$: s7	$C_{51}H_{98}O_6$: g23 $C_{57}H_{104}O_6$: g22
C ₂₇ H ₁₉ NO: b148 C ₂₇ H ₄₂ CINO ₂ : b33	C ₃₀ H ₆₃ O ₃ P: t308 C ₃₂ H ₆₆ : d737	

TABLE 1.15 Physical Constants of Organic Compounds See also the special tables of fats, oils, and waxes.

Names of the compounds in the table starting on p. 1.82 are arranged alphabetically. Usually substitutive nomenclature is employed; exceptions generally involve ethers, sulfides, sulfones, and sulfoxides. Each compound is given a number within its letter classification; thus compound c195 is 3-chlorophenol. The section "Nomenclature of Organic Compounds" should be consulted to familiarize oneself with present nomenclature systems.

Synonyms or Alternate Names are found at the bottom of each spread in their alphabetical listing; the number following the name refers to the numerical place of this compound in the table. For example, epichlorohydrin, c101, indicates that this compound is found listed under the name 1-chloro-2,3-epoxypropane.

Formulas are presented in a semistructural form when no ambiguity is possible. Complicated systems are drawn in complete structural form and located at the bottom of each page and keyed to the number of the entry.

Beilstein Reference. In the column so headed is found the reference to the volume and page numbers of the fourth edition of Beilstein: (Handbuch der Organischen Chemie) (Springer-Verlag, New York). Thus the entry 9, 202 refers to an entry in volume 9 appearing on page 202. When the volume number has a superscript attached, reference is made to the appropriate supplementary volume. For example, 12², 404 indicates that the compound will be found listed in the second supplement to volume 12 on page 404. The earliest Beilstein entry is listed. Supplementary information may be found in the supplements to the basic series; such coordinating references (series number, volume number, and page number of the main edition) along with the system number are found at the top of each *odd-numbered* page. Similarly, a back reference such as H 93; E II 64; E III 190 in a volume of Supplementary Series IV means that previous items on

TABLE 1.14 Empirical Formula Index for Organic Compounds (continued)

C ₂₄ H ₅₁ O ₃ P: d423, t421 C ₂₄ H ₅₂ O ₄ Si: t85 C ₂₄ H ₅₄ OSn ₂ : b201	C ₂₇ H ₄₆ O: c262 C ₂₇ H ₅₀ ClN: b94	C ₃₂ H ₆₈ O ₄ Si: t86 C ₃₆ H ₇₅ O ₃ P: d642 C ₃₈ H ₃₀ NiO ₂ P ₂ : b213 C ₃₀ H ₇₄ O ₆ : g20
C ₂₆	C ₂₈ C ₂₈ H ₂₇ : t129	C ₃₀ H ₇₄ O ₆ , g20 C ₄₀ H ₅₆ : c19 C ₄₀ H ₈₂ O ₆ P ₂ : b196
C ₂₆ H ₂₀ : t131 C ₂₆ H ₂₆ N ₂ O ₂ S: b152	C ₂₈ H ₃₂ C ₁ Si ₃ : r2 C ₂₈ H ₃₂ O ₂ Si ₃ : t121	C ₄₅ to C ₅₇
C ₂₆ H ₂₆ OSi ₂ : t130 C ₂₆ H ₅₀ O ₄ : b177, d311	C ₃₀ to C ₄₀	C ₄₅ H ₈₆ O ₆ : g24 C ₄₈ H ₄₀ O ₄ Si ₄ : o38
	$C_{30}H_{50}$: s8 $C_{30}H_{62}$: s7	$C_{51}H_{98}O_6$: g23 $C_{57}H_{104}O_6$: g22
C ₂₇ H ₁₉ NO: b148 C ₂₇ H ₄₂ CINO ₂ : b33	C ₃₀ H ₆₃ O ₃ P: t308 C ₃₂ H ₆₆ : d737	

TABLE 1.15 Physical Constants of Organic Compounds See also the special tables of fats, oils, and waxes.

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this compound are found in the same volume of the Basic Series on page 93, of Supplementary Series II on page 64, and of Supplementary Series III on page 190. The absence of a back reference implies that the compound involved is described for the first time in the series concerned.

Formula Weights are based on the International Atomic Weights of 1973 and are computed to the nearest hundredth.

Density values are given at room temperature unless otherwise indicated by the superscript figure: thus 0.9711¹¹² indicates a density of 0.9711 for the substance at 112°C. A density of 0.899¹⁶ indicates a density of 0.899 for the substance at 16°C relative to water at 4°C.

Refractive Index, unless otherwise specified, is given for the sodium line at 589.6 nm. The temperature at which the measurement was made is indicated by the superscript figure; otherwise it is assumed to be room temperature.

Melting Point is recorded in certain cases as 250 d and in some other cases as d 250, the distinction being made in this manner to indicate that the former is a melting point with decomposition at 250 °C, while the latter decomposition occurs only at 250°C and higher temperatures. Where a value such as -2H₂O₂, 120 is given, it indicates a loss of 2 mol of water per formula weight of the compound at a temperature of 120°C.

Boiling Point is given at atmospheric pressure (760 mmHg) unless otherwise indicated; thus 82^{15 mm} indicates that the boiling point is 82 °C when the pressure is 15 mmHg. Also, subl 550 indicates that the compound sublimes at 550 °C.

Flash Point is given in degrees Celsius, usually closed up. Because values will vary with the specific procedure employed, and sometimes the method was not stated, the values listed for the flash point should be considered only as indicative. See also Table 4.13. Properties of Combustible Mixtures in Air.

Solubility is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent and at room temperature. Other temperatures are indicated by the superscript. In the case of gases, the solubility is often expressed as 510° mL, which indicates that at 10 °C, 5 mL of the gas is soluble in 100 g of the solvent.

Abbreviations Used in the Table

EtOH, ethanol, 95%

expl, explodes

pyr, pyridine

abs, absolute acet, acetone alc, ethanol alk, alkali (i.e., aqueous NaOH or KOH) anhyd, anhydrous aq, aqueous; water as, asymmetrical atm, atmosphere BuOH, butanol hz benzene c, cold chl, chloroform, CHCl3 conc, concentrated d, decomposes or decomposed d(+), dextrorotatory $-d_n$, deuterium substitution D, designates configuration delig, deliquescent dil, dilute diox, dioxane DL (or dl), inactive (i.e., 50% D and 50% L)

DMF, dimethylformamide EtAc, ethyl acetate eth, diethyl ether

glyc, glycerol h. hot HOAc, acetic acid hyd, hydrolysis hygr, hygroscopic i, insoluble ign, ignites i-PrOH, isopropanol 1 (−), levorotatory L, designates configuration m, meta position Me, methyl MeEtKe, methyl ethyl ketone MeOH, methanol misc, miscible; soluble in all proportions NaOH, aqueous sodium

hydroxide o, ortho position org, organic p, para position PE, petroleum ether

s, soluble sec, secondary sl, slight or slightly soln, solution solv, solvent subl, sublimes s, symmetrical sym, symmetrical tert, tertiary v, very v s, very soluble v sl s, very slightly soluble vac, vacuo or vacuum

vols, volumes >, greater than <, less than ~, approximately α , alpha position β , beta position y, gamma position δ , delta position ε , epsilon position

 ω , omega position (farthest from parent functional group)

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a1	(-)-Abietic acid		302.44	92, 424	_		172–175			i aq; s alc, bz, chl, eth, acet, dil alk
a2	Acenaphthene		154.21	5, 586	1.069_{95}^{95}		93.45	279		i aq; 3.2 alc; 20 bz
a3	Acenaphthlyene		152.20	5, 625	0.899_4^{16}		80–83	280		i ag; v s alc, eth
a4	Acetaldehyde	CH₃CHO	44.05	1,594	0.8053_4^0	1.3311^{20}	-123.5	20.2	-27	misc aq, alc
a5	Acetaldoxime	CH ₃ CH=NOH	59.07	1,608	0.966	1.415^{20}	46.5	114.5	38	v s aq, alc; eth
a6	Acetamide	CH ₃ CONH ₂	59.07	2^2 , 177	0.9711112	1.4158110	80.1	221.15		70 aq; 50 alc; s chl, hot bz
a7	Acetamidine HCl	CH ₃ (=NH)NH ₂ ·HCl	94.54	2, 185			170–172			v s aq, alc; i acet, eth
a8	N-(2-Acetamido)- 2-aminoethane- sulfonic acid	H ₂ N(CO)CH ₂ NHCH ₂ - CH ₂ SO ₃ H	182.20				>220 d			
a9	4-Acetamidobenz- aldehyde	CH₃CONHC₀H₄CHO	163.18	14, 38			154–156			s aq, bz; sl s alc
a10	4-Acetamidobenzene- sulfonyl chloride	CH ₃ CONHC ₆ H ₄ SO ₂ Cl	233.67	14, 439			149			d aq; v s alc, eth
a11	2-Acetamidobenzoic acid	CH₃CONHC₀H₄COOH	179.18	14, 337			185–187			sl s aq; v s alc, bz, eth, acet
a12	4-Acetamidobenzoic acid	CH₃CONHC₀H₄COOH	179.18	14, 432			260–262			i aq; s alc; sl s eth
a13	2-Acetamidofluorene		223.28	12, 1331			194			i aq; s alc, glycols
a14	N-(2-Acetamido)- iminodiacetic acid	H ₂ NCOCH ₂ N(CH ₂ COOH) ₂	190.16	·			219 d			
a15	2-Acetamidophenol	CH₃CONHC₀H₄OH	151.17	13, 370			207-209			
a16	3-Acetamidophenol	CH ₃ CONHC ₆ H ₄ OH	151.17	13, 415			146-149			
a17	4-Acetamidophenol	CH₃CONHC₀H₄OH	151.17	13, 460	1.293_4^{21}		170			s alc, acet
	I	I	I	I		I	l		I	l

a18	Acetanilide	CH ₃ CONHC ₆ H ₅	135.17	12, 237	1.219_4^{15}		114.2	304	173	0.56 aq ²⁵ ; 29 alc;
										2bz; 27 chl; 25
					20					acet; 5 eth
a19	Acetic acid	CH₃COOH	60.65	2,96	1.0492_4^{20}	1.3716^{20}	16.63	117.90	40	misc aq, alc, eth,
										CCl ₄
a20	Acetic acid-d	CH ₃ COOD	61.05		1.07	1.3715^{20}		115.5	40	misc aq, alc, eth,
		-								CCl ₄
a21	Acetic-d ₃ , acid-d	CD₃COOD	64.08		1.11	1.3709^{20}		115.5	40	misc aq, alc, eth
a22	Acetic anhydride	(CH ₃ CO) ₂ O	102.09	2, 166	1.082_4^{15}	1.3904^{20}	-73.1	140.0	130	13 aq; s chl, eth
a23	Acetic anhydride-d ₆	(CD ₃ CO) ₂ O	108.14			1.3875^{20}		65 ^{65mm}	54	d aq, alc
a24	Acetoacetic acid	CH3COCH2COOH	102.09	3,630			36–37	d violently		misc aq, alc, eth
								100		_
a25	Acetohydrazide	CH ₃ CONHNH ₂	74.08	2, 191				129 ^{18mm}		
a26	Acetone	CH ₃ COCH ₃	58.08	1,635	0.7908_4^{20}	1.3588^{20}	-95.35	56.24	-20	misc aq, alc, chl,
a27	Acetone-d ⁶	CD ₃ COCD ₃	64.13		0.88	1.3554^{20}		55.5	-17	-
a28	Acetone oxime	$(CH_3)_2C$ =NOH	73.10	1,649	0.901		60-63	135		v s aq, alc, eth

ACES, a8 Acetal, d251 Acetaldehyde ammonia, a163 Acetaldehyde diethyl acetal, d251 Acetaldehyde dimethyl acetal, d438 Acetamidoacetic acid, a46 2-Acetamidopentanedioic acid, a45 Acethydrazide, a25 Acetic acid hydrazide, a25 Acetoacetanilide, a32 2-Acetoacetanisidide, a302 4-Acetoacetanisidide, a303 Acetoacetic esters, e53, e54 Acetoin, h106 Acetonaphthones, m311, m312 Acetonecarboxylic acid, a24 Acetone cyanohydrin, h145 Acetone dimethyl acetal, d452 Acetone dimethyl acetal, d452 Acetone ketal of glycerine, d515

a1

a3

a13

a2

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a29 a30 a31 a32	Acetonitrile Acetonitrile-d ₃ Acetophenone 2-Acetylacetanilide	CH ₃ CN CD ₃ CN C ₆ H ₃ COCH ₃ C ₆ H ₃ NHCOCH ₂ COCH ₃	41.05 44.08 120.15 177.20	2, 183 7, 271 12, 518	0.7857 ²⁰ 0.84 1.0238 ²⁵	1.3441 ²⁰ 1.3420 ²⁰ 1.5322 ²⁵	-43.8 19.62 85	81.60 80.7 202.08	5 5 82	misc aq, alc, chl misc aq, alc, chl 0.55 aq; s alc, eth sl s aq; s alc, hot bz, chl, eth, acids, alk
a33	4-Acetylbenzene- sulfonic acid, Na salt	CH ₃ COC ₆ H ₄ SO ₃ ⁻ Na ⁺	222.02	11 ² , 186			>300			uorus, urk
a34	4-Acetylbiphenyl	C ₆ H ₅ C ₆ H ₄ COCH ₃	196.25	$7^2,337$			116–118	325–327		i ag; v s alc, acet
a35	Acetyl bromide	CH₃COBr	122.95	2, 174	1.66346		-96	75–77	1	d aq, alc; misc bz, chl, eth
a36	2-Acetylbutyrolactone		128.13		1.1846_4^{20}	1.4585^{20}		107 ^{5mm}		21 aq
a37	Acetyl chloride	CH₃COCl	78.50	2, 173	1.104420	1.3886 ²⁰	-112.9	50.8	4	d aq, alc; misc bz, chl, eth
a38	Acetylcholine bromide	(CH ₃) ₃ NBrCH ₂ CH ₂ — OCOCH ₃	226.14	41, 428			114–116			v s aq (d hot aq); s alc; i eth
a39	Acetylcholine chloride	(CH ₃) ₃ NClCH ₂ CH ₂ — OCOCH ₃	181.66	4, 281			150–152			v s aq; alc; d hot aq; i eth
a40	2-Acetylcyclo- pentanone		126.16	7,558	1.043	1.4905^{20}		72–75 ^{80mm}	72	•
a41	Acetylene	НС≡СН	26.02	1, 228	0.90(g)		-81 ^{891mm}	-83.95 subl		90 aq; 14 alc; v s bz, eth; acet dissolves 25 acet ^{15°}
a42	Acetylenedicarboxylic acid	HOOCC≡ CCOOH	114.06	2, 801			180 d			v s aq, alc, eth
a43	Acetyl fluoride	CH₃COF	62.04	2, 172	1.032		>-60	20		5 aq(d); misc alc, bz, eth

a44	2-Acetylfuran		110.11	17, 286	1.098	1.5065 ²⁰	29–30	67 ^{10mm}	71	
a45	N-Acetyl-L- glutamic acid	HOOCCH ₂ CH ₂ CH— (NHCOCH ₃)COOH	189.17	$4^2,908$			200–201			
a46	N-Acetylglycine	CH ₃ CONHCH ₂ COOH	117.10	4, 354			207–209			2.7 aq ¹⁵ ; s alc; i eth
a47	N-Acetylimidazole		110.12				93–96			
a48	Acetyl iodide	CH₃COI	169.96	2, 174	2.0674_4^{20}	1.5491^{20}		108		d aq, alc; s bz, eth
a49	Acetyl-2-methyl- choline chloride	CH ₃ COOCH(CH ₃)CH ₂ - NC1(CH ₃) ₃	195.69				171–173			v s aq, alc, chl; i eth
a50	2-Acetylphenothiazine	7 2/2	241.31				180-185			
a51	2-Acetylphenylaceto- nitrile	C ₆ H ₅ CH(CN)COCH ₃	159.19	10, 699			89–92			
a52	N-Acetyl-		141.17		1.146	1.5026^{20}		218	>112	
	4-piperidone									

Acetonylacetone, h61 Acetophenetidin, e45 Acetophenetidide, e45 p-Acetotoluide, m355 Acetoxime, a28 2-Acetoxybenzoic acid, a56

1-Acetoxy-1,3-butadiene, b375

Aceturic acid, a46 Acetylacetaldehyde dimethyl acetal, d435 Acetylacetone, p31 N-Acetylanthranilic acid, a11 Acetylbenzene, a31 Acetylcyclopropane, c368 Acetylene dichlorides, d179, d180

Acetylene tetrabromide, t9 Acetylene tetrachloride, t28 N-Acetylethanolamine, h115 3-Acetyl-6-methyl-2*H*-pyran-2,4-(3*H*)-dione, d21 2-(Acetyloxy)benzoic acid, a56

3-Acetyl-1-propanol, h157

a44

a50

a52

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a53 a54	2-Acetylpyridine 3-Acetylpyridine	(C ₅ H ₄ N)COCH ₃ (C ₅ H ₄ N)COCH ₃	121.14 131.14	21, 279 21, 279	1.080 1.102	1.5203 ²⁰ 1.5336 ²⁰		188–189 220	>112 150	v s alc, eth v s acids, alc, eth; s aq
a55 a56	4-Acetylpyridine Acetylsalicyclic acid	(C ₅ H ₄ N)COCH ₃ HOOCC ₆ H ₄ OOCCH ₃	121.14 180.16	21, 279 10, 67	1.095 1.35	1.5290 ²⁰	135	212	>112	0.33 aq ²⁵ ; 20 alc; 5.9 chl; 5 eth; sl s bz
a57	2-Acetylthiophene	(C ₄ H ₃ S)COCH ₃	126.18	17, 287	1.168422	1.5564 ²⁰	10–11	214		sl s aq; misc alc, eth
a58	<i>N</i> -Acetylthiourea	CH ₃ CONHC(S)NH ₂	118.16	3, 191			165–169			s hot aq, alc; sl s eth
a59	N-Acetyl-DL-		246.27	22², 469			204–206			s aq, alc; v s eth
a60	tryptophan Acid alizarin violet N		366.33	16 ² , 127						
a61	Acridine		179.22	20, 459			107–110 subl	346		s alc, eth, CS ₂ , PE
a62	Acrylamide	H ₂ C=CHCONH ₂	71.08	2,400	1.122 ³⁰		110 84.5	125 ^{25mm}		215 aq ³⁰ ; 86 alc ³⁰ ; 63 acet; 2.7 chl; v s eth
a63	Acrylic acid	H ₂ C=CHCOOH	72.06	2, 397	1.051120	1.4224 ²⁰	13	140–141	54	misc aq, alc, bz, eth, chl, acet
a64	Acrylonitrile	H ₂ C=CHCN	53.06	2,400	0.8060_4^{20}	1.3911 ²⁰	-83.7	77.4	0	7.3 aq; misc org
a65 a66	Acryloyl chloride 1-Adamantanamine	H ₂ C=CHCOCI	90.51 151.25	2,400	1.114	1.4350 ²⁰	206–208	72–76	16	d aq; v s chl sl s aq
a67	Adamantane		136.24		1.09	1.568	268 sealed tube	subl 205		

a68	1-Adamantane- carboxylic acid
a69	Adenine
a70	Adenosine

180.25		
135.13	26, 420	
267.25	31, 27	

174–175		
>360 d	subl 220	0.05 a
234–236		chl, s aq; i

aq; sl s alc; i l, eth alc

N-Acetylsulfanilyl chloride, a10 Aconitic acid, p207 Acrolein, p204

Acrolein diethyl acetal, d258 Acrolein dimethyl acetal, d454 Acrylaldehyde, p207

1-Adamantanemethylamine, a209 Adenosine monophosphate, a72





TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a71	Adenosine-5'-diphos- phoric acid		427.22							
a72	Adenosine-5'- phosphoric acid		347.22				200 d			v s hot aq, HC1
a73	D-α-Alanine	CH ₃ CH(NH ₂)COOH	89.09	4, 385			291-293 d			
a74	DL-α-Alanine	CH ₃ CH(NH ₂)COOH	89.09	4, 387	1.402		289 d	subl		16.7 aq ²⁵ ; 8.7 alc ²⁵ ; i eth
a75	L-α-Alanine	CH ₃ CH(NH ₂)COOH	89.09	4, 381			315–316			16.7 aq ²⁵ ; 8.7 alc ²⁵ ; i eth
a76	β-Alanine	H,NCH,CH,COOH	89.09	4, 401	1.437-5		197-198 d			v s aq; sl s alc; i eth
a77	Allantoin		158.12	25, 474			238			0.45 aq; 0.2 alc
a78	Allene	H ₂ C=C=CH ₂	40.06	1, 248	1.787	1.4168	-136.2	-34.5		1
a79	Alloxan monohydrate		160.09	24, 500			253 d			s alc, acet, HOAc; sl s chl, PE, EtAc
a80	Allyl acetate	H ₂ C=CHCH ₂ OCOCH ₃	100.12	2, 136	$0.928^{0.928}_{4}$	1.4040^{20}		104	6	i aq; misc alc, eth
a81	Allyl alcohol	H ₂ C=CHCH ₂ OH	58.08	2, 436	0.8540_4^{20}	1.4127^{20}	−50 glass	97.1	22	misc aq, alc, chl,
a82	Allylamine	H ₂ C=CHCH ₂ NH ₂	57.10	4, 205	0.760_{20}^{20}	1.4205^{20}	-88.2	53.3	-28	misc aq, alc, chl, eth
a83	N-Allylaniline	$C_6H_5NHCH_7CH=CH_7$	133.19	12, 170	0.982^{25}	1.5630^{20}		218-220	89	i aq; s alc, eth
a84	Allylbenzene	$C_6H_5CH_2CH=CH_2$	118.18	5, 484	0.892_0^{20}	1.5122^{20}		156-157	33	i aq; s alc, eth
a85	Allyl bromide	H ₂ C=CHCH ₂ Br	120.98	1, 201	1.45125	1.465^{25}	-50	70	7	i aq; misc org solv
a86	Allylchlorodimethyl- silane	H_2C =CHC H_2 Si- (C H_3) ₂ C1	134.7		0.89642	1.4195^{20}		110–112		
a87	Allyl chloroformate	H ₂ C=CHCH ₂ OOCC1	120.54		1.13	1.423		27	31	

a88 a89	Allylcyclohexylamine Allyldichloromethyl-	C ₆ H ₁₁ NHCH ₂ CH=CH ₂ H ₂ C=CHCH ₂ Si-	139.24 155.1		$0.962 \\ 1.0758^{20}$	$1.4664^{20} \\ 1.4419^{20}$		66 ^{12mm} 119–120	53	
	silane	(CH ₃)Cl ₂								
a90	N-Allyl-N,N-	$H_2C = CHCH_2N(CH_3)_2$	85.0			1.4010^{20}		63-64		
	dimethylamine									
a91	Allyl ethyl ether	$H_2C = CHCH_2OCH_2CH_3$	86.13	1,438	0.7651_4^{20}	1.388120		64–66		i aq; misc alc, eth
a92	Allyl iodide	H_2C = $CHCH_2I$	167.98	1, 202	1.846_4^{20}		-99.3	103.1		i aq; misc alc, eth

Adenosine 5'-(trihydrogen diphosphate), a71 5'-Adenylic acid, a72 Adipic acid, h57 Adipic acid monoethyl ester, e149 Adiponitrile, d238 Adipolyl chloride, h62 ADP, a71 Alaninols, a271, a272 Alizarin, d371 Allylacetic acid, p50 Allylacetone, h78 4-Allylanisole, a94 Allyl carbamide, a105 Allyl chloride, c216

Allyl cyanide, b400 Allyldimethylchlorosilane, a86 Allyl glycidyl ether, a96 1-Allyl-2-hydroxybenzene, a98 Allyl iodide, i50

a71

1.89

a72

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a93	Allyl isothiocyanate	H ₂ C=CHCH ₂ NCS	99.16	4, 214	1.013420	1.5300 ²⁰	-80	150	46	0.2 aq; misc org
a94	1-Allyl-4- methoxybenzene	H ₂ C=CHCH ₂ C ₆ H ₄ OCH ₃	148.21	6, 571	0.9645421	1.5195 ²⁰		215–216		a slc, chl
a95	Allyl methyl sulfide	H ₂ C=CHCH ₂ SCH ₃	88.17	1,440	0.803	1.4714^{20}		91–93	18	
a96	1-Allyloxy- 2,3-epoxypropane	H_2C — $CHCH_2OCH_2$ O CH = CH_2	114.14		0.962	1.433220		154	57	
a97	Allyloxytrimethyl- silane	H_2C = $CHCH_2OSi(CH_3)_3$	130.3		0.7830	1.4075 ²⁵		100–101		
a98	2-Allylphenol	H ₂ C=CHCH ₂ C ₆ H ₄ OH	134.18	6, 572	1.025515	1.545520	-6	220	88	s alc, eth
a99	Allyl phenyl ether	$H_2C = CHCH_2OC_6H_5$	134.18	6, 144	0.98345	1.5200 ²⁰		192	62	i aq; s alc; misc eth
a100	Allyl propyl ether	$H_2C = CHCH_2OC_3H_7$	100.16	1 ³ , 1882	0.7670_4^{20}	1.3919^{20}		90–92	38	s alc; misc eth
a101	1-Allyl-2-thiourea	H_2C = $CHCH_2NHC(S)NH_2$	116.18	4, 211	1.219_{20}^{20}		78			3.3 aq; s alc; i bz; v sl s eth
a102	Allyltrichlorosilane	H ₂ C=CHCH ₂ SiCl ₃	175.5		1.2011420	1.4460^{20}		117.5		
a103	Allyltriethoxysilane	$H_2C = CHCH_2Si - (OC_2H_5)_3$	204.3		0.9030^{20}	1.4072 ²⁰		176 ^{740mm}		
a104	Allyltrimethylsilane	$H_2C = CHCH_2Si(CH_3)_3$	114.27		0.7193_4^{20}	1.4074^{20}		85–86	7	
a105	Allylurea	$H_2C = CHCH_2NHCONH_2$	100.12	4, 209			78	15		v s aq, alc; v sl s eth
a106	Aminoacetonitrile	H ₂ NCH ₂ CN	56.07	4, 344				58 ^{15mm} d		s acids, alc
a107	Aminoacetonitrile hydrogen sulphate	H ₂ NCH ₂ CN·H ₂ SO ₄	154.14	4, 344			101	d 165		v s aq; sl s alc; i eth
a108	2'-Aminoaceto- phenone	H ₂ NC ₆ H ₄ COCH ₃	135.17	14, 41				70 ^{3mm}		v sl s aq; s alc, eth
a109	3'-Aminoaceto- phenone	H ₂ NC ₆ H ₄ COCH ₃	135.17	14, 45			98–99	289–290		
a110	4'-Aminoaceto- phenone	H ₂ NC ₆ H ₄ COCH ₃	135.17	14, 46			106	293–295		s hot aq, alc, eth, HOAc; sl s bz

a111	1-Aminoanthra- quinone		223.23	14, 177	
a112	2-Aminoanthra- quinone		223.23	14, 191	
a113	4-Aminoantipyrine		203.25	24, 273	
a114	2-Aminobenzamide	H ₂ NC ₆ H ₄ CONH ₂	136.15	14, 320	
a115	2-Aminobenzene- arsonic acid	H ₂ NC ₆ H ₄ AsO(OH) ₂	217.06	16 ¹ , 463	
a116	4-Aminobenzene- arsonic acid	$H_2NC_6H_4AsO(OH)_2$	217.06	16, 878	
a116a	5-Aminobenzene-1,3- dicarboxylic acid	H ₂ NC ₆ H ₃ (COOH) ₂	181.15	14 ¹ , 636	
a117	2-Aminobenzene-1,4- disulfonic acid	$H_2NC_6H_3(SO_3H)_2$	253.24		
a118	2-Aminobenzene- sulfonic acid	H ₂ NC ₆ H ₄ SO ₃ H	173.19	14, 681	

253–255 295 d	subl	i aq; v s alc, bz, chl, eth, HOAc, HCl i aq, eth; s alc, bz
109		s aq, alc, bz; sl s
110	300 sl d	v s hot aq, alc; i bz; sl s eth
153		02, 31 3 Cui
>300		s hot aq, alk CO ₃ ,
>300		mineral acids
d 325		1.5 aq ¹⁵ ; v sl s alc,
		eth

Allyl mercaptan, p206

4-Allyl-2-methoxyphenol, m99

2-Allyl-4-methylphenol, m387

2-Allyl-6-methylphenol, m386

Allyl sulfide, d27 Aluminon, a316

N-Amidinosarcosine, c277

Aminoacetaldehyde diethyl acetal, d254

Aminoacetaldehyde dimethyl acetal, d440 1-Aminoadamantane, a66 Aminoanisoles, m42, m43, m44 *p*-Aminoazobenzene, p87

a113

.9

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a119	3-Aminobenzene- sulfonic acid	H ₂ NC ₆ H ₄ SO ₃ H	173.19		1.69					2 aq ¹⁵ ; sl s alc
a120	4-Aminobenzene- sulfonic acid	H ₂ NC ₆ H ₄ SO ₃ H	173.19	14, 695			d 288			1 aq ²⁰ ; sl s hot MeOH
a121	2-Aminobenzoic acid	H ₂ NC ₆ H ₄ COOH	137.14	14, 310			144-146	subl		v s hot aq, alc, eth
a122	3-Aminobenzoic acid	H ₂ NC ₆ H ₄ COOH	137.14	14, 383	1.5114		172–174			sl s aq; v s alc; s eth
a123	4-Aminobenzoic acid	H ₂ NC ₆ H ₄ COOH	137.14	14, 418	1.374		187			0.59 aq; 5.6 alc
a124	2-Aminobenzonitrile	H ₂ NC ₆ H ₄ CN	118.14	14, 322			49	268		s alc, eth
a125	3-Aminobenzonitrile	H ₂ NC ₆ H ₄ CN	118.14	14, 391			53	288–290		s hot aq; v s alc, eth
a126	4-Aminobenzonitrile	H ₂ NC ₆ H ₄ CN	118.14	14, 425			85	d		v s hot aq, alc, eth
a127	2-Aminobenzo- phenone	H ₂ NC ₆ H ₄ COC ₆ H ₅	197.24	14, 76			108	223–226		sl s aq; s alc, eth
a128	2-Aminobenzothiazole		150.20	27, 182			132	d		v s alc, chl, eth
a129	2-Aminobenzotri- fluoride	H ₂ NC ₆ H ₄ CF ₃	161.13	12 ² , 453	1.290 ²⁵	1.4785 ²⁵	34	175	55	
a130	3-Aminobenzotri- fluoride	H ₂ NC ₆ H ₄ CF ₃	161.13	12, 870	1.290	1.480020	6	187	85	
a131	4-Aminobenzotri- fluoride	H ₂ NC ₆ H ₄ CF ₃	161.13	12 ³ , 2151	1.283 ²⁷	1.4815 ²⁵	38	107 ^{39mm}	85	
a132	N-(p-Aminobenzoyl)- glycine	H ₂ NC ₆ H ₄ CONHCH ₂ COOH	194.19	14 ² , 258			198–199			i aq; s alc, bz, chl
a133	4-Aminobenzoyl hydrazide	H ₂ NC ₆ H ₄ CONHNH ₂	151.17	14 ¹ , 570			227			
a134	2-Aminobiphenyl	$H_2NC_6H_4C_6H_5$	169.23	12, 1317			53	299		sl s aq; s alc
a135	4-Aminobiphenyl	$H_2NC_6H_4C_6H_5$	169.23	12, 1318			54	191 ^{15mm}		s hot aq, alc, eth
a136	D-(+)-2-Amino-1- butanol	CH ₃ CH ₂ CH(NH ₂)CH ₂ OH	89.14	4, 291	0.947 ²⁰	1.4521 ²⁰	-2	174	79	misc aq; s alc

a137	L-(-)-2-Amino-1-	CH ₃ CH ₂ CH(NH ₂)CH ₂ OH	89.14	4, 291	0.947^{20}	1.4525^{20}	-2	174	82	misc aq; s alc
a138	butanol DL-2-Aminobutyric acid	CH ₃ CH ₂ CH(NH ₂)COOH	103.12	4, 408			304	subl 300		21 aq; 0.2 hot alc
a139	4-Aminobutyric acid	H ₂ NCH ₂ CH ₂ COOH	103.12	4,413			195.d			v s aq; i alc, eth
a140	2-Amino-4-chloro- benzoic acid	H ₂ N(Cl)C ₆ H ₃ COOH	171.58	14, 365			233			
a141	2-Amino-5-chloro- benzonitrile	H ₂ N(Cl)C ₆ H ₃ CN	152.58				99	132 ^{0.5mm}	>112	
a142	2-Amino-4'-chloro- benzophenone	H ₂ NC ₆ H ₄ COC ₆ H ₄ Cl	231.68	14 ¹ , 389			104			
a143	2-Amino-5-chloro- benzophenone	H ₂ N(Cl)C ₆ H ₃ COC ₆ H ₅	231.68	14, 79			100			
a144	2-Amino-5-chloro- benzotrifluoride	H ₂ N(Cl)C ₆ H ₃ CF ₃	195.57	12³, 1921	1.386	1.5069^{20}		66–67 ^{3mm}		
a145	3-Amino-4-chloro- benzotrifluoride	H ₂ N(Cl)C ₆ H ₃ CF ₃	195.57		1.428	1.4975 ²⁵		82-83 ^{9mm}	none	
a146	5-Amino-2-chloro- benzotrifluoride	H ₂ N(Cl)C ₆ H ₃ CF ₃	195.57				36			

Aminobenzenethiol, a293 Aminobenzoic acid hydrazide, a133 Aminobenzyl cyanide, a260 1-Aminobutane, b417 2-Aminobutane, b377 Aminobutanoic acids, a138, a139 3-Amino-2-butenamide, a150 4-Aminobutyraldehyde diethyl acetal, d247 α -Aminocaproic acid, a183 ε -Aminocaproic acid, a184

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a147	2-(3-Amino-4-chloro- benzoyl)benzoic acid	H ₂ N(Cl)C ₆ H ₃ CO- C ₆ H ₄ COOH	275.69	14, 661			171–173			
a148	2-Amino-4-chloro- phenol	H ₂ N(Cl)C ₆ H ₃ OH	143.57	13, 383			138			
a149	2-Amino-5-chloro- pyridine	$H_2N(Cl)C_5H_3N$	128.56	22 ² , 332			138	128 ^{11mm}		
a150	3-Aminocrotamide	$CH_3C(NH_2) = CHCONH_2$	100.12				102			
a151	3-Aminocrotononitrile	$CH_3C(NH_2)$ =CHCN	82.11	3,660						
a152	1-Amino-1-cyclo-	C ₆ H ₁₀ (NH ₂)COOH	143.19	14, 299			>300			
	hexanecarboxylic acid									
a153	5-Amino-2,3-dihydro- 1,4-phthalazine- dione		177.16	25 ¹ , 698			319–320			
a154	2-Amino-4,6-dihy- droxypyrimidine		127.10	24, 468			>300			
a155	4-Amino-2,6-dihy- droxypyrimidine		127.10	24, 469			>300			
a156	4-Amino-3,5-diiodo- benzoic acid	I ₂ (NH ₂)C ₆ H ₂ COOH	388.93	14, 439			>300			i aq, alc
a157	2-Amino-4,6-di- methylpyridine	$(CH_3)_2(NH_2)(C_5H_2N)$	122.17	22, 435			64	235		
a158	4-Amino-2,6-di- methylpyridimide		123.16	$24^2, 45$			181			156 aq; 18.9 alc
a159	6-Amino-1,3-di- methyluracil		155.16	24, 471			295 d			
a160	5-Amino-2,6-dioxo- 1,2,3,6-tetrahydro-		171.11	25, 264			>300			
	4-pyrimidinecar- boxylic acid									

a161	2-Aminoethane-	H ₂ NCH ₂ CH ₂ SO ₃ H	125.15	4, 528			d > 300			6.45 aq ¹² ; i abs alc
	sulfonic acid									
a162	2-Aminoethanethiol	HSCH ₂ CH ₂ NH ₂	77.14	4, 286			99–100			v s aq; s alc
a163	1-Aminoethanol	CH ₃ CH(OH)NH ₂	61.08				97	110 d		s aq; sl s eth
a164	2-Aminoethanol	H ₂ NCH ₂ CH ₂ OH	61.08	4, 274	1.0158^{20}	1.4539^{20}	10.52	171	93	misc aq, org solv
a165	2-(2-Aminoethoxy)-	H ₂ NCH ₂ CH ₂ OCH ₂ CH ₂ OH	105.14	$4^3,642$	1.460			218–224		
	ethanol									
a166	2-(2-Aminoethyl-	H ₂ NCH ₂ CH ₂ NHCH ₂ -	104.15	4, 286	1.030	1.4861^{20}		241	129	v s aq, alc; sl s eth
	amino)ethanol	CH ₂ OH								
a167	5-(2-Aminoethyl-	H ₂ NCH ₂ CH ₂ NH-	266.32				>300			
	amino)-1-naphtha-	$C_{10}H_6SO_3H$								
	lenesulfonic acid									
a167a	3-(2-Aminoethyl-	H ₂ NCH ₂ CH ₂ NHCH ₂ CH ₂ -	222.1		1.01_4^{25}	1.4418^{25}		140 ^{15mm}	150	
	amino)propyl-	CH ₂ Si(OCH ₃) ₃								
	trimethoxy-									
	silane									

4-Amino-*m*-cresol, a218 Aminocyclohexane, c334 Aminodecane, d19

2-Amino-2-deoxyglucose, g5

2-Amino-5-diethylaminopentane, d327

2-Amino-1,5-dihydro-1-methyl-4 *H*-imidazol-4-one, c278

2-Aminodiphenylamine, p131

1-Amino-1,2-diphenylethane, d668

Aminodiphenylmethane, d678

Aminoethane, e58 1-(2-Aminoethyl)amino-2-[(2-aminoethyl)aminoethyl]aminoethane, t54

$$\begin{array}{c|c} & NH_2 \\ \hline N & \\ H_3C & N \end{array} CH_3$$

a159

a153

a154

a155

a158

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a168	3-Amino-9-ethyl-		210.28	221, 642			98–100			
a169	carbazole 2-Aminoethyl hydrogen sulfate	H ₂ NCH ₂ CH ₂ OSO ₃ H	141.15	4, 276			280 d			
a170	3-(2-Aminoethyl)- indole		160.22	221,636			118	137 ^{0.15mm}		i aq, bz, chl, eth; s alc, acet
a171	S-2-Aminoethyl- isothiouronium bromide HBr		281.02				194–195			s are, acer
a172	N-(2-Aminoethyl)- morpholine		130.19		0.992	1.4755 ²⁰	25.6	205	175	
a173	p-(2-Aminoethyl)- phenol	HOC ₆ H ₄ CH ₂ CH ₂ NH ₂	137.18	13, 625			161–163	175 ^{8mm}		
a174	N-(2-Aminoethyl)- piperazine		129.21		0.985	1.4983 ²⁰	-26	222	93	
a175	N-(2-Aminoethyl)- 1,3-propanediamine	H ₂ NCH ₂ CH ₂ CH ₂ NHCH ₂ - CH ₂ NH ₂	117.20		0.928	1.4815 ²⁰			96	
a176	2-Amino-2-ethyl-1,3- propanediol	HOCH ₂ C(NH ₂) - (C ₂ H ₅)CH ₂ OH	119.16		1.099_{20}^{20}	1.49020	38	152 ^{10mm}	74	misc aq; s alc
a177	2-(2-Aminoethyl)- pyridine	$H_2NCH_2CH_2(C_5H_4N)$	122.17	22, 434	1.021	1.5357 ²⁰		93 ^{12mm}		
a178	4-(2-Aminoethyl)- pyridine	$H_2NCH_2CH_2(C_5H_4N)$	122.17		1.012	1.5403 ²⁰		104 ^{9mm}		
a179	3-Amino-4- fluorobenzo- trifluoride	H ₂ N(F)C ₆ H ₃ CF ₃	179.0			1.4608 ²⁰		81 ^{20mm}		
a180	Aminoguanidine H ₂ CO ₃	$H_2NNHC(=NH) - NH_2 \cdot H_2CO_3$	136.11	3, 117			172 d			i aq; d hot aq

a181 a182	Aminoguanidine nitrate N-Aminohexamethyl-	$H_2NNHC(=NH)-NH_2 \cdot HNO_3$ $C_6H_{12}N=NH_2$	137.11	3, 117	0.984	1.4850 ²⁰	137	165	56	
4102	eneimine	6111214 14112	114.17		0.704	1.4050		103	30	
a183	2-Aminohexanoic acid	CH ₃ (CH ₂) ₃ CH(NH ₂)-	131.18	4, 433	1.172		d 327			1.15 aq ²⁵ ; 0.42 alc
		СООН								
a184	6-Aminohexanoic acid	H ₂ N(CH ₂) ₄ CH ₂ COOH	131.18	4, 434			204-206			v s aq; i alc
a185	6-Amino-1-hexanol	H ₂ N(CH ₂) ₅ CH ₂ OH	117.19	$4^2,748$			56-58	135 ^{30mm}		
a186	1-Amino-4-hydroxy-		239.23	14, 268			207-209			s eth
	anthraquinone									
a187	L-2-Amino-3-hydroxy-	CH₃CH(OH)CH-	119.12	4, 514			d 255-			v s aq; i alc, eth,
	butyric acid	(NH ₂)COOH					257			chl

Aminoethylbenzenes, e64, e65 2-(2-Aminoethyl)-2-thiopseudourea, a171

1-Aminoheptane, h20

2-Aminoheptane, m269a

1-Aminohexane, h80

2-Aminohexane, m353a

p-Aminohippuric acid, a132 Aminohydroxybenzoic acids, a286, a287

a172

$$\begin{bmatrix} h_{3} \dot{N} C H_{2} C H_{2} S C \\ N H_{2} \end{bmatrix} 2 B r^{-}$$

$$C H_{2} C H_{2} N H_{2}$$

$$a 171$$

$$a 172$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a188	DL-2-Amino-4- hydroxy- butyric acid	HOCH ₂ CH ₂ CH- (NH ₂)COOH	119.12	4, 514			188–189			s alc
a189	L-2-Amino-4-hydroxy- butyric acid	HOCH ₂ CH ₂ CH- (NH ₂)COOH	119.12	4 ³ , 1636			203 d			
a190	DL-4-Amino-3- hydroxy- butyric acid	H ₂ NCH ₂ CH(OH)- CH ₂ COOH	119.12	4 ² , 938			202 d			s aq; sl s alc, eth
a191	4-Amino-6-hydroxy-2- mercapto- pyrimidine hydrate		161.18	24, 476			>300			
a192	2-Amino-4-hydroxy-6- methylpyrimidine		125.13	24, 343			>300			
a193	4-Amino-3-hydroxy-1- naphthalenesulfonic acid		239.25	14, 846			295 d			i aq, alc, bz, eth
a194	4-Amino-5-hydroxyl-1- naphthalenesulfonic acid		239.25	14, 835						sl s aq; i alc, eth
a195	5-Amino-6-hydroxy-2- naphthalenesulfonic acid		239.25							sl s hot aq; i eth
a196	6-Amino-7-hydroxy-2- naphthalenesulfonic acid		239.25	14, 849			>300			
a197	2-Amino-3-hydroxy- pyridine	$H_2N(HO)(C_5H_3N)$	110.12	22 ² , 408			172–174			
a198	4-Amino-2-hydroxy- pyrimidine		111.10	24, 314			>300			0.77 aq; sl s alc

100	1 4 · · · · · · · · · · · · · · · · · ·	1	122.10	10 1101	1 02015	1.561220	115	0.78mm	0.4	l 1
a199	1-Aminoindan		133.19	12, 1191	1.038_4^{15}	1.5613^{20}	1.5	97 ^{8mm}	94	sl s aq
a200	5-Aminoindan		133.19	12 ¹ , 511			36	249 ^{745mm}		sl s aq
a201	5-Aminoindazole		133.15	$25^2,308$			178			
a202	6-Aminoindazole		133.15	25, 317			206 d			
a203	2-Amino-5-iodoben-	H ₂ N(I)C ₆ H ₃ COOH	263.03	14, 373			221 d			sl s aq, PE; s alc
	zoic acid									
a204	DL-2-Amino-4-mer-	HSCH ₂ CH ₂ CH-	135.19	4 ³ , 1647			232-233			
	captobutyric acid	(NH ₂)COOH								
a205	Aminomethane-	H ₂ NCH ₂ SO ₃ H	111.12	1,583			185 d			v s aq
	sulfonic acid									

2-Amino-2-(hydroxymethyl)-1,3-propanediol, t423

 α -Amino-4-imidazolepropanoic acid, h83

Aminoiminomethanesulfinic acid, f30

N-(Aminoiminomethyl)-N-methylglycine, c277

2-Aminoisobutyric acid, a222

5-Aminoisophthalic acid, a116a

6-Amino-2,4-lutidine, a157

2-Amino-3-mercaptopropanoic acid, c370

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a206	3-Amino-4-methoxy- benzoic acid	CH ₃ O(NH ₂)C ₆ H ₃ COOH	167.16	14 ¹ , 657			241			
a207	2-Amino-6-methoxy- benzothiazole		180.23	27 ² , 334			165–167			
a208	5-Amino-2-methoxy- pyridine	CH ₃ O(NH ₂)C ₅ H ₃ N	124.14	22 ² , 408		1.5745 ²⁰	31	90 ^{1mm}		
a209	1-(Aminomethyl)- adamantane		165.28		0.933	1.5137 ²⁰		83–85 ^{0.3 mm}	92	
a210	4-(Aminomethyl)- benzenesulfonamide	H ₂ NCH ₂ C ₆ H ₄ SO ₂ NH ₂	186.25				151–152			s dil alk, dil acid
a211	2-Amino-5-methyl- benzoic acid	H ₂ N(CH ₃)C ₆ H ₃ COOH	151.17	14, 481			177 d			sl s aq; s alc, eth
a212	3-Amino-4-methyl- benzoic acid	H ₂ N(CH ₃)C ₆ H ₃ COOH	151.17	14, 487			166			a aq
a213	DL-2-Amino-3-methyl- 1-butanol	(CH ₃) ₂ CHCH(NH ₂)- CH ₂ OH	103.17			1.4543 ²⁰		77 ^{8mm}	83	
a214	L-2-Amino-3-methyl- 1-butanol	(CH ₃) ₂ CHCH(NH ₂)- CH ₂ OH	103.17		0.926	1.4548 ²⁰		81 ^{8mm}	78	
a215	2-(Aminomethyl)- 1-ethylpyrrolidine	-	128.22		0.887	1.4665 ²⁰		60 ^{16mm}		
a216	2-Amino-3-methyl- 1-pentanol	CH ₃ CH ₂ CH(CH ₃)CH- (NH ₂)CH ₂ OH	117.19			1.4589 ²⁰	30	97 ^{14mm}		
a217	2-Amino-4-methyl- 1-pentanol	CH ₃ CH(CH ₃)CH ₂ CH- (NH ₂)CH ₂ OH	117.19	4, 298	0.917	1.4511 ²⁰		200	90	
a218	4-Amino-3-methyl- phenol	H ₂ N(CH ₃)C ₆ H ₃ OH	123.16	13, 593			179			
a219	4-(Aminomethyl)- piperidine		114.19			1.4900 ²⁰	25	200	78	
a220	2-Amino-2-methyl- 1,3-propanediol	HOCH ₂ C(CH ₃)- (NH ₂)CH ₂ OH	105.14	4, 303			110	151 ^{10mm}		250 aq ²⁰ ; s alc

a221	2-Amino-2-methyl- 1-propanol	(CH ₃) ₂ C(NH ₂)CH ₂ OH	89.14		0.934_{20}^{20}	1.4480 ²⁰	30–31	165	67	misc aq; s alc, org
a222	2-Amino-2-methyl- propionic acid	(CH ₃) ₂ C(NH ₂)COOH	103.12	4, 414			335 sealed tube	280 subl		v s aq
a223	2-(Aminomethyl)- pyridine	$H_2NCH_2(C_5H_4N)$	108.14		1.049	1.5445 ²⁰	1400	85 ^{12mm}		
a224	3-(Aminomethyl)- pyridine	$H_2NCH_2(C_5H_4N)$	108.14		1.062	1.5510^{20}	-21	74 ^{1mm}	100	
a225	2-Amino-3-methyl- pyridine	$H_2N(CH_3)(C_5H_3N)$	108.14	22 ² , 342		1.578220	34	222		v s aq; s alc
a226	2-Amino-4-methyl- pyridine	$H_2N(CH_3)(C_5H_3N)$	108.14	22 ² , 342			100	230		v s aq, alc, DMF
a227	2-Amino-6-methyl- pyridine	$H_2N(CH_3)(C_5H_3N)$	108.14	221, 633			45	209		v s aq
a228	2-Amino-4-methyl- pyrimidine		109.13	24, 84			160	subl		s hot aq; s alc
a229	2-Amino-4-methyl- thiazole		114.17	27, 159			45	232		v s aq, alc, eth
a230	2-Aminomethyl-3,5,5- trimethylcyclo-		171.29		0.969	1.4904 ²⁰	43–48	265	>112	
	hexanol			l	1					

1-Amino-2-methoxyethane, m69 α -(Aminomethyl)benzyl alcohol, a262

3-Amino-α-methylbenzyl alcohol, a261

2-Amino-3-methylpentanoic acid, i79

2-Aminomethylthiophene, t158

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a231 a232	N-Aminomorpholine 2-Amino-1, 5-naph- thalenedisulfonic acid		102.14 303.31	27, 8 14, 786	1.059	1.4772 ²⁰	>300	168	58	
a233	7-Amino-1,3-naph- thalenedisulfonic acid		303.31	14, 784			>300			
a234	4-Amino-1-naph- thalenesulfonic acid	$H_2NC_{10}H_6SO_3H$	223.26		1.670425		d			0.031 aq; s dil alk
a235	4-Amino-1,8-naph- thalimide		212.21	$22^2, 452$			360			
a236	3-Amino-2-naphthol	$H_2NC_{10}H_6OH$	159.19	13,685			207			
a237	2-Amino-4-nitro- benzoic acid	H ₂ N(NO ₂)C ₆ H ₃ COOH	182.14	14, 374			270 d			i aq; v s alc, eth
a238	2-Amino-5-nitro- benzonitrile	$H_2N(NO_2)C_6H_3CN$	163.14	14 ² , 234			200–207			
a239	2-Amino-5-nitro- benzophenone	$C_6H_5COC_6H_3$ - $(NH_2)NO_2$	242.23	14, 79			166–168			
a240	2-Amino-6-nitro- benzothiazole		195.20	27 ² , 232			247–249			
a241	2-Amino-5-nitro- benzotrifluoride	$H_2N(NO_2)C_6H_3CF_3$	206.12				90–92			
a242	4-Amino-3-nitro- benzotrifluoride	$H_2N(NO_2)C_6H_3CF_3$	206.12				105–106			
a243	4-Amino-4'-nitro- diphenylsulfide	O ₂ NC ₆ H ₄ SC ₆ H ₄ NH ₂	246.29	13, 534			142			
a244	2-Amino-4-nitro- phenol	O ₂ N(NH ₂)C ₆ H ₃ OH	154.13	13 ² , 192			145			

a245	4-Amino-2-nitro-	$O_2N(NH_2)C_6H_3OH$	154.13	13,520			127			
	phenol									
a246	D-(-)-threo-2-Amino-	HOCH ₂ CH(NH ₂)CH(OH)-	212.21				163–165			
	1-(<i>p</i> -nitrophenyl)-	$C_6H_4NO_2$					163–165			
	1,3-propanediol									
a247	2-Amino-5-(p-nitro-		285.30				222-226			
	phenylsulfonyl)-									
	thiazole									
a248	2-Amino-5-nitro-	$H_2N(C_5H_3N)NO_2$	139.11	221, 631			188			sl s aq, bz, eth
	pyridine									
a249	2-Amino-5-nitro-		145.14				202 d			v sl s aq; 0.7 alc;
	thiazole									0.4 eth
a250	exo-2-Aminonorbor-		111.19		0.938	1.4807^{20}		49 ^{10mm}	35	
	nane									

1-Aminonaphthalene, n17

1-Amino-2-naphthol-4-sulfonic acid, a193

1-Amino-2-naphthol-6-sulfonic acid, a195

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a251 a252	2-Aminopentane 3-Aminopentane	H(CH ₂) ₃ CH(NH ₂)CH ₃ C ₂ H ₅ CH(NH ₂)C ₂ H ₅	87.17 87.17	4, 177 4, 178	$0.739^{20} \\ 0.749^{20}_{4}$	1.4047 ²⁰ 1.4055 ²⁰		91–92 91	1	s aq, alc, eth, PE misc aq, alc, eth
a253	DL-2-Aminopentanoic acid	H(CH ₂) ₃ CH(NH ₂)COOH	117.15	4,416			303	320 subl		5.5 aq ¹⁸ ; v sl s alc, chl, eth, PE
a254	5-Aminopentanoic acid	H ₂ N(CH ₂) ₄ COOH	117.15	4, 418			158–161			v s aq; sl s alc; i eth
a255	5-Amino-1-pentanol	H ₂ N(CH ₂) ₅ OH	103.17	4 ¹ , 441 13 ³ , 1679	1.045	1.4615^{20} 1.5849^{20}	37	122 ^{16mm} 148 ^{4mm}	65 >112	
a256	2-Aminophenethyl alcohol	H ₂ NC ₆ H ₄ CH ₂ CH ₂ OH	137.18	13°, 16/9	1.045	1.5849-		148	>112	
a257	2-Aminophenol	H ₂ NC ₆ H ₄ OH	109.13	13, 354			170–174			2 aq; 4.3 alc; v s eth; sl s bz
a258	3-Aminophenol	H ₂ NC ₆ H ₄ OH	109.13	13, 401			122-123	164 ^{11mm}		2.5 aq; v s alc, eth
a259	4-Aminophenol	H ₂ NC ₆ H ₄ OH	109.13	13, 427			190	284 d		0.65 aq; s alc, eth
a260	4'-Aminophenylaceto- nitrile	H ₂ NC ₆ H ₄ CH ₂ CN	132.17	14, 457			44	312		sl s hot aq; s alc
a261	1-(3-Aminophenyl)- ethanol	H ₂ NC ₆ H ₄ CH(CH ₃)OH	137.18	13 ³ , 1654			68–71			
a262	2-Amino-1-phenyl- ethanol	C ₆ H ₅ CH(CH ₂ NH ₂)OH	137.18	13 ² , 361			56–57	160 ^{17mm}		v s aq; s alc
a263	1S,2S-(+)-2-Amino- 1-phenyl-1,3-pro- panediol	C ₆ H ₅ CH(OH)CH(NH ₂)- CH ₂ OH	167.21				109–113			
a264	L-2-Amino-3-phenyl-	C ₆ H ₅ CH ₂ CH(NH ₂)-	151.21	13 ³ , 1757			92–94			
	1-propanol	CH ₂ OH								
a265	3-Amino-1-phenyl-	_	175.19				210-215			
	2-pyrazolin-5-one									
a266	N-Aminophthalimide		162.15				200–202			
a267	N-Aminopiperidine		100.17	20, 89	0.928	1.4750^{20}		146 ^{730mm}	36	
a268	3-Amino-1,2-pro-	H ₂ NCH ₂ CH(OH)CH ₂ OH	91.11	4, 301	1.175	1.4920^{20}		265 ^{739mm}	>112	
	panediol									

a269	DL-1-Amino-2-	CH ₃ CH(OH)CH ₂ NH ₂	75.11	4, 289	0.973	1.4483^{20}	-2	160	73	s aq, alc; i eth
	propanol									•
a270	DL-2-Amino-1-	CH ₃ CH(NH ₂)CH ₂ OH	75.11	4 ¹ , 432	0.943	1.4495^{20}		173–176		v s aq, alc, eth
	propanol									
a271	L-2-Amino-1-propanol	CH ₃ CH(NH ₂)CH ₂ OH	75.11	4 ¹ , 432	0.965	1.4495^{20}		176	62	v s aq, alc, eth
a272	3-Amino-1-propanol	H ₂ NCH ₂ CH ₂ CH ₂ OH	75.11	4, 288	0.982	1.4598^{20}	12	188	79	s aq, alc
a273	2-Amino-1-propene-	$NCC(CN) = C(NH_2)$ -	132.13				171-173			s aq
	1,1,3-tricarbonitrile	CH ₂ CN								_
a274	3-Aminopropionitrile	H ₂ NCH ₂ CH ₂ CN	70.09					185		
a275	3-Aminopropyl-	$H_2N(CH_2)_3Si(CH_3)$ -	191.4		0.916_4^{20}	1.427^{20}		85–88 ^{8mm}		
	(diethoxy)methyl-	(OCH ₂ CH ₃) ₂								
	silane									
a276	N-(3-Aminopropyl)-	H ₂ N(CH ₂) ₃ N-	162.23		0.1071	1.4980^{20}		170 ^{2mm}	137	
	iminodiethanol	(CH ₂ CH ₂ OH) ₂								
a277	N-(3-Aminopropyl)-		144.22		0.9872_{20}^{20}	1.4761^{20}	-15	224	98	misc ag, alc, bz
	morpholine				20					1, ,
a278	N-(3-Aminopropyl)-2-		142.20		1.014	1.5000^{20}		120-	>112	
	pyrrolidinone							123 ^{1mm}		
	1 1 2					l .	I .		1	

5-Aminoorotic acid, a160

1-Aminopentane, p53

4-Aminophenyl phenyl ether, p70 Aminophenyl sulfones, d36, d37 3-Aminophthalhydrazide, a153 Aminopicolines, a225, a226, a227 1-Aminopropane, p220

2-Aminopropane, i88

3-Amino-1-propene, a82 *N*-(3-Aminopropyl)diethanolamine, a276

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a279	3-Aminopropyl- triethoxysilane	H ₂ N(CH ₂) ₃ Si(OC ₂ H ₅) ₃	221.37		0.9506420	1.4225 ²⁰		217	96	
a280	3-Aminopropyl- trimethoxysilane	H ₂ N(CH ₂) ₃ Si(OCH ₃) ₃	179.2		1.0125	1.420 ²⁵		80 ^{8mm}	104	
a281	2-Aminopyridine	$(C_5H_4N)NH_2$	94.12	22, 428			58.1	210.6	92	s aq, alc, bz, eth
a282	3-Aminopyridine	$(C_5H_4N)NH_2$	94.12	22, 431			64	248		s aq, alc, bz, eth
a283	4-Aminopyridine	(C ₅ H ₄ N)NH ₂	94.12	22, 433			155–158	273		s aq, alc; sl s bz, eth
a284	2-Aminopyrimidine		95.11	24, 80			123-126	subl		v s aq
a285	4-Aminoquinaldine		158.20	22, 453			169	333		sl s aq; v s alc, eth, acet; s hot bz
a286	4-Aminosalicyclic acid	H ₂ NC ₆ H ₃ (OH)COOH	153.14	14, 579			147 d			0.2 aq; 4.8 alc; s dil acid, alk
a287	5-Aminosalicyclic acid	H ₂ NC ₆ H ₃ (OH)COOH	153.14	14, 579			280 d			sl s aq, alc; s acid
a288	2-Amino-3-sulfopropionic acid	HOOCCH(NH ₂)- CH ₂ SO ₃ H	187.17	4, 533			260 d			v s aq
a289	5-Amino-1,2,3,4-tetr- azole hydrate		103.08	26, 403			204 d			
a290	5-Amino-1,3,4-thia- diazole-2-thiol		133.20	27,674			235 d			
a291	2-Aminothiazole		100.14	27, 155			93			sl s aq, alc, eth
a292	2-Amino-2-thiazole		100.14	27, 136			91-93			-
a293	2-Aminothiophenol	H ₂ NC ₆ H ₄ SH	125.19	13, 397		1.6405^{20}	26	234	79	
a294	6-Amino-3-toluene-	H ₂ NC ₆ H ₃ (CH ₃)SO ₃ H	187.22	14, 723			>300			1 aq ¹² ; v s hot aq
	sulfonic acid									
a295	3-Amino-1,2,4-		84.08	26, 137			159			s aq, alc, chl
	triazole									

a296	5-Amino-2,2,4-tri- methyl-1-cyclopent- anemethylamine		156.27		0.901	1.4733 ²⁰		221	97	
a297	11-Aminoundecanoic acid	$H_2N(CH_2)_{10}COOH$	201.31				190–192			
a298	Aniline	$C_6H_5NH_2$	93.13	12, 59	1.0217 ²⁰	1.5855 ²⁰	-5.98	184.40	70	3.5 aq ²⁵ ; s alc, CCl ₄ , eth, acids
a299	Aniline hydrochloride	C ₆ H ₄ NH ₂ ·HCl	129.59		1.222		198		193	100 aq; v s alc
a300	2-Anilinoethanol	C ₆ H ₅ NHCH ₂ CH ₂ OH	137.18	12, 182	1.085	1.5793^{20}		150-	>112	sl s ag; v s alc, chl,
								152 ^{10mm}		eth
a301	3-Anilinopropio-	C ₆ H ₅ NHCH ₂ CH ₂ CN	146.19				52-53			
	nitrile									

6-Aminopurine, a69

2-Amino-3-pyridinol, a197

Aminopyrimidinediols, a154, a155

2-Aminosuccinamic acid, a313

Aminosuccinic acid, a314

6-Amino-2-thiouracil, a191

 α -Amino-p-toluenesulfonamide, a210

2-Amino-1,1,3-tricyanopropene, a273

1-Aminotricyclo[3.3.1.1^{3,7}]decane, a66

Aminouracil, a155

2-Aminovaleric acid, a253

5-Aminovaleric acid, a254

Amyl compounds, see Pentyl

Amyl alcohol, p37

act-Amyl alcohol, m153

sec-Amyl alcohol, p38

tert-Amyl alcohol, m154

tert-Amylamine, d601

Amyl bromides, b322, b323

Amyl chloride, c191

Amyl iodide, i47

Amyl mercaptan, p35

Amyl methyl ketone, h15

Anethole, m97

Angelic acid, m162

Anilinesulfonic acids, a118, a119, a120

Aniline-2,5-disulfonic acid, a117

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a302	1-(o-Anisidino)-1,3- butanedione	CH ₃ OC ₆ H ₄ NHCOCH ₂ - COCH ₃	207.23	13¹, 117			84–85			
a303	1-(<i>p</i> -Anisidino)-1,3- butanedione	CH ₃ OC ₆ H ₄ NHCOCH ₂ - COCH ₃	207.23	13 ¹ , 177			115–117			
a304	Anthracene	3	178.23	5, 657	1.25 ²⁷ ₄		216.3	340		i aq; 1.5 alc; 1.6 bz; 1.2 chl; 3.1 CS ₂
a305	9,10-Anthracene- dione		208.22	7, 781	1.43 ²⁰		286	377	185	i aq; 0.44 alc; 0.26 bz; 0.61 chl; 0.11 eth
a306	9,10-Anthraquinone- 1,5-disulfonic acid disodium salt		412.31	11, 340			>300			s aq
a307	9,10-Anthraquinone- 2,6-disulfonic acid disodium salt		412.31	11, 342			>325			s aq
a308	9,10-Anthraquinone- 2-sulfonic acid Na salt		310.26							
a309	Antipyrine		188.23	24, 27	1.0884113		114	319 ^{174mm}		100 aq; 77 alc; 100 chl; 2.3 eth
a310	L-(+)-Arabinose		150.13	31, 32			160-163			100 aq
a311	L-(+)-Arginine	H ₂ NC(=NH)NH(CH ₂) ₃ - CH(NH ₂)COOH	174.20	4, 420			223 d			17.6 aq; sl s alc
a312	L-(+)-Ascorbic acid	-	176.12				190– 192 d			100 aq; 3.3 alc
a313	L-(+)-Asparagine hydrate	H ₂ NCOCH ₂ CH(NH ₂)- COOH·H ₂ O	150.14	4, 484			233–235			3.6 aq ²⁸ ; s alk acids; i alc, bz, eth

a314	L-(+)-Aspartic acid	HOOCCH ₂ CH(NH ₂)COOH	133.10	4, 472		270		0.45 aq; i alc, eth
						sealed		
						tube		
a315	Atropine		289.38	21, 27		114-116		0.22 aq; s bz, dil
								acid

Anisaldehydes, m45, m46 Anisamide, m47 Anisic acids, m50, m51, m52 Anisidines, m42, m43, m44 Anisole, m48 p-Anisoyl chloride, m53

p-Anisyl alcohol, m54 Anthraflavic acid, d374 Anthranilamide, a114 Anthranilic acid, a121 Anthranionitrile, a124 9,10-Anthraquinone, a305 APDC, p271 Araboascorbic acid, i59 Aspirin, a56 Arsanilic acids, a115, a116

a310

a312

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a316	Aurintricarboxylic acid, triammonium salt		473.44	10 ² , 775			225 d			v s aq
a317 a318	2-Azacyclooctanone 2-Azacyclotri- decanone		127.19 197.32	21, 242			35–38 150–153	148 ^{10mm}		
a319 a320 a321 a322	Azidotrimethylsilane Azidotriphenylsilane 1-Aziridineethanol cis-Azobenzene	$(CH_3)_3SiN_3$ $(C_6H_5)_3SiN_3$ $(CH_2)_2$ =NCH ₂ CH ₂ OH C_6H_5N =NC ₆ H ₅	115.21 301.4 87.12 182.23	16, 8	0.868 1.088 1.20	1.4142^{20} 1.4560^{20}	-95 83-84 68.3	95–96 100 ^{0.01mm} 168 293	23 67	i aq; s alc, eth,
a323	2,2'-Azobis(2-methyl)- propionitrile	(CH ₃) ₂ C(CN)N=N- C(CN)(CH ₃) ₂	164.21	4, 563				107 d		HOAc 2 EtOH; 5 MeOH; can explode in acetone
a324 a325	Azodicarbonamide 4,4'-Azoxydianisole	$H_2NCON = NCONH_2$ $CH_3OC_6H_4N = N(\rightarrow O)$ - $C_6H_4OCH_3$	116.08 258.28	3, 123 16, 637			225 d 120			
a326	Azulene		128.17	52, 432			100.5	250		
b1	Barbituric acid		128.09	24, 467			248– 252 d			s hot aq, dil acid
b2 b3	Basic fuchsin Benzaldehyde	C ₆ H ₅ CHO	337.86 106.12	13, 765 7, 174	1.22 1.0447 ²⁰	1.5455 ²⁰	d 186 -26	178.9	62	0.3 aq; s alc, acids 0.3 aq; misc alc, eth
b4	Benzamide	C ₆ H ₅ CONH ₂	121.14	9, 195	1.3414		127.2	288		1.3 aq; 17 alc; 30 pyr
b5	Benzanilide	C ₆ H ₅ CONHC ₆ H ₅	197.24	12, 262	1.315		163.1	117 ^{10mm}		i aq; 1.7 alc; sl s
b6	1,2-Benzanthracene		228.29	5,718			155–157	437.6		sl s hot alc; s most other org solv

b7 b8	2,3-Benzanthracene 7 <i>H</i> -Benz[<i>de</i>]- anthracen-7-one		228.29 230.27	5 ² , 628 7, 518	1.35		341 170	subl		sl s most org solv 1.6 bz; 0.5 HOAc
b8a	Benzene	C_6H_6	78.11	5, 179	0.8737 ²⁵	1.4979 ²⁵	5.53	80.10	-11	0.17 aq; s most org
b9 b10	Benzene- <i>d</i> Benzene- <i>d</i> ₆	C_6H_5D C_6D_6	79.12 84.16		0.95	$1.4980^{20} \\ 1.4978^{20}$		80 79.1	-11 -11	

Azacyclopropane, e131 Azelaic acid, n95 Azelonitrile, n94 Aziridine, e131 Azobis(isobutyronitrile), a323 4,4'-Azoxyanisole, a325 Barbitol, d280 Behenic acid, d716 Behenyl alcohol, d717 Benzalacetone, p96 Benzal bromide, d102 Benzalphthalide, b101 Benzanthrone, b8 Benzeneacetaldehyde, p76a

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b11 b12	Benzenearsonic acid Benzeneboronic acid	C ₆ H ₅ AsO(OH) ₂ C ₆ H ₅ B(OH) ₂	202.04 121.93	16, 868 16, 920	1.760 ²⁵		163 d 217 to the anhy- dride	-H ₂ O on standing in air		2.5 aq; 2 alc 2.6 aq; 1.8 alc; 43 eth; s bz
b13	1,4-Benzenedicarb- aldehyde	C ₆ H ₄ (CHO) ₂	134.13	7, 675			114	248		i aq; 6 bz; 17 acet; 2 eth; 14 diox; 46 MeOH
b14	1,3-Benzendi- carbonyl dichloride	C ₆ H ₄ (COCl) ₂	203.02	9, 834			43–44	276	180	73 bz; 62 CCl ₄
b15	1,4-Benzenedi- carbonyl dichloride	C ₆ H ₄ (COCl) ₂	203.02	9, 844			81	266	180	37 bz; 9 CCl ₄
b16	1,3-Benzenedicar- boxylic acid	$C_6H_4(COOH)_2$	166.13	9, 832			345–348	subl		0.012 aq; v s alc, HOAc; i bz, PE
b17	1,4-Benzendicar- boxylic acid	C ₆ H ₄ (COOH) ₂	166.13	9, 841			subl without melting			v sl s aq, chl, eth; sl s alc; s alk
b18	1,4-Benzenedi- methanol	$C_6H_4(CH_2OH)_2$	138.17	6, 919	1.10017		115	1431mm	188	v s aq, alc, eth
b19	Benzenehexacar- boxylic acid	C ₆ (COOH) ₆	342.17	9, 1008			286 d			v s aq, alc
b20	Benzenesulfinic acid	$C_6H_5S(=O)OH$	142.16	11, 2			85	100 d		sl s aq; s alc, bz, eth
b21	Benzenesulfonamide	C ₆ H ₅ SO ₂ NH ₂	157.19	11, 39			152			i aq; sl s alc; s eth
b22	Benzenesulfonic acid	C ₆ H ₅ SO ₂ OH	158.18	11, 26			50-51			v s aq, alc; sl s bz
b23	Benzenesulfonyl chloride	C ₆ H ₅ SO ₂ Cl	176.62	11, 34	1.384215	1.5518	14.5	177 ^{100mm}	>112	i aq; s alc, eth
b24	Benzenesulfonyl fluoride	C ₆ H ₅ SO ₂ F	160.16	11 ² , 23	1.3286 ₄ ²⁰	1.493218		203–204		s alc, eth

b25	Benzenesulfonyl hydrazide	C ₆ H ₅ SO ₂ NHNH ₂	172.21	11, 52	101–103		flammable solid
b26	1,2,4,5-Benzenetetra- carboxylic acid	C ₆ H ₂ (COOH) ₄	254.15	9, 997	276		1.5 aq; v s alc
b27	1,2,4,5-Benzenetetra- carboxylic anhydride		218.12	19, 196	283–286	397–400	
b28	1,2,3-Benzenetricar- boxylic acid dihydrate	C ₆ H ₃ (COOH) ₃ ·2H ₂ O	246.18	9,976	192 d		sl s aq; v s eth
b29	1,2,4-Benzenetricar- boxylic acid	C ₆ H ₃ (COOH) ₃	210.14	9,977	321 d		2.1 aq; 25.3 alc; 7.9 acet; v s eth
b30	1,3,5-Benzenetricar- boxylic acid	C ₆ H ₃ (COOH) ₃	210.14	9, 978	>330		sl s aq; v s alc; s eth
b31	1,2,4-Benzenetricar- boxylic anhydride		192.13	18, 468	161–164	245 ^{14mm}	50 acet; 22 EtAc

Benzeneazobenzene, a322 Benzenecarbonitrile, b51 Benzene-1,2-dicarboxylic acid, p167 Benzenemethanol, b78 Benzenethiol, t159

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b32	1,3,5-Benzenetricar-	C ₆ H ₃ (COCl) ₃	265.48				35–36			
	boxylic trichloride									
b33	Benzethonium chloride	(CH ₃) ₃ CCH ₂ C(CH ₃) ₂ - C ₆ H ₄ OCH ₂ CH ₂ OCH ₂ - CH ₂ N ⁺ (CH ₃) ₂ - CH ₂ C ₆ H ₅ Cl ⁻	448.10				164–166			v s aq; s alc, acet
b34	Benzil	C ₆ H ₅ COCOC ₆ H ₅	210.23	7, 747	1.23_4^{15}		94.9	346		i aq; s alc, eth
b35	Benzil- α -dioxime	$C_6H_5C(=NOH)C(=NOH)$								11
1.26	D '11' '1	C ₆ H ₅	220.25	10.242			152			s alk
b36	Benzilic acid	(C ₆ H ₅) ₂ C(OH)COOH	228.25	10, 342			153			sl s aq; v s alc, eth
b37 b38	Benzil monohydrazone Benzimidazole	$C_6H_5C(=NNH_2)COC_6H_5$	224.26 118.14	7 ¹ , 394 23, 131			150–152 170.5	>360		-1411-
b39	Benzimidazoie Benzo-15-crown-5		268.3	23, 131			76–78	>300		sl s aq, eth; v s alc
b40	7,8-Benzo-1,3-diaza- spiro-[4,5]decane-		216.24				268–270			
	2,4-dione		4044			4.5.40.520		4.0.26mm	0.7	
b41	1,4-Benzodioxan		136.15		1.142	1.5485 ²⁰		103 ^{6mm}	87	
b42	2,3-Benzofuran		118.14	17,54	1.072	1.5660 ²⁰	<-18	175		i aq; misc bz, eth, PE
b43	Benzofurazan-1-oxide		136.11	271, 740			69-71			
b44	Benzoic acid	C ₆ H ₅ COOH	122.13	9,92	1.080		122.4	132.5 ^{10mm}	121	0.29 aq; 43 alc; 10 bz; 22 chl; 33 eth; 33 acet
b45	Benzoic anhydride	$(C_6H_5CO)_2O$	226.23	9, 164	1.199		39–40	360		i aq; s alc, acet, chl, bz, HOAc
b46	DL-Benzoin	C ₆ H ₅ COCHOHC ₆ H ₅	212.25	8, 165	1.3100^{20}_{4}		134–136	344		s acet; 20 pyr
b47	Benzoin ethyl ether	C ₆ H ₅ CH(OC ₂ H ₅)- COC ₆ H ₅	240.30	8, 174	$1.1016_4^{\overline{17}}$	1.5727 ¹⁷	61	195 ^{20mm}		s alc, bz, eth

b48	Benzoin isobutyl	C ₆ H ₅ CH[OCH ₂ CH-	268.36		0.985	1.5485^{20}		133 ^{0.5mm}	85	
	ether	$(CH_3)_2]COC_6H_5$								
b49	Benzoin methyl ether	C ₆ H ₅ CH(OCH ₃)COC ₆ H ₅	226.28	8, 174	1.1278_4^{14}		48	189 ^{15mm}		v s alc, bz, eth
b50	α-Benzoinoxime	$C_6H_5CH(OH)C(=NOH)$ -	227.26	8, 175			151-152			sl s aq; s alc,
		C ₆ H ₅								NH ₄ OH
b51	Benzonitrile	C ₆ H ₅ CN	103.12	9, 275	1.0006^{25}	1.5257^{25}	-12.75	191.1	71	0.2 aq; misc alc,
										bz, chl, eth
b52	Benzo[def]phen-		202.26	5, 693	1.271^{23}			156	404	i aq; s alc, eth
	anthrene									1
b53	Benzophenone	C ₆ H ₅ COC ₆ H ₅	182.22	7,411	1.1108_4^{15}		48.1	305		i aq; 13.3 alc;
										17 eth
b54	Benzophenone	$C_6H_5C(=NNH_2)C_6H_5$	196.25	7,417			98	230 ^{55mm}		
	hydrazone									

Benzhydrazide, b72 Benzhydrol, d677 Benzhydrylamine, d678 Benzhydryl bromide, b274 Benzidine, b136

b39

2-Benzimidazolethiol, m15 1,3-Benzodiazole, b38 1,3,2-Benzodioxaborole, c21 1,3-Benzodioxole, m240 Benzofuroxan, b43 Benzoglyoxaline, b38 Benzoic acid hydrazide, b72 *o*-Benzoic sulfimide, s1

TABLE 1.15 Physical Constants of Organic Compounds (continued)

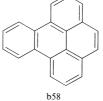
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b55	3,3',4,4'-Benzophen- onetetracarboxylic dianhydride		322.23				215–217			
b56	1-Benzopyran-4(4 <i>H</i>)		146.15	17, 327			55–57			
b57 b58	1,2-Benzo[<i>a</i>]pyrene 4,5-Benzo[<i>e</i>]pyrene		252.32 252.32		20		179.3 182	495		i aq; s bz; sl s alc i aq
b59	1,4-Benzoquinone	O=C ₆ H ₄ =O	108.10	7,609	1.318420		115.7			sl s aq; s alc, eth, hot bz, alk (with d)
b60	Benzothiazole		135.19		1.246_4^{20}	1.6379^{20}	2	231	>112	sl s aq; v s alc, CS ₂
b61	Benzo[b]thiophene		134.20	17, 59	1.193740	1.630240	31.32	221		s alc, bz, chl, eth
b62	1,2,3-Benzotriazole		119.13	26, 38	1.238	1.6420 ²⁰	98.5	204 ^{15mm}		sl s aq; s alc, bz, chl
b63	Benzoxazole		119.12	27, 42		1.5594	30	182	58	sl s aq
b64	1-Benzoylacetone	C ₆ H ₅ COCH ₂ COCH ₃	162.19	7,680	1.090^{60}_{60}		60	260 sl d		sl s aq; v s alc, eth
b65	2-Benzoylbenzoic acid	C ₆ H ₅ COC ₆ H ₄ COOH	226.23	10, 747			129	265		sl s aq; v s alc, eth
b66	Benzoyl bromide	C ₆ H ₅ COBr	185.03	9, 195	1.546720	20		218–219	90	d aq, alc; misc eth
b67	Benzoyl chloride	C ₆ H ₅ COCl	140.57	9, 182	1.21120	1.5525 ²⁰	-1.0	197.2	68	d aq, alc; misc bz, CS ₂ , eth
b68	Benzoyl cyanide	C ₆ H ₅ COCN	131.13	10, 659			32	206		i aq
b69	Benzoyl fluoride	C ₆ H ₅ COF	124.11	9, 181	1.140	1.4960 ²⁰	-28	161	48	d hot aq; v s alc, eth
b70	Benzoylformic acid	C ₆ H ₅ COCOOH	150.13	10, 654			69			
b71	N-Benzoylglycine	C ₆ H ₅ CONHCH ₂ COOH	179.18	9, 225			178–179			0.4 aq; 0.1 chl; 0.25 eth; sl s alc; i bz, PE
b72	Benzoylhydrazine	C ₆ H ₅ CONHNH ₂	136.15	9, 319			117			

b73	3-Benzoylpropionic acid	C ₆ H ₅ COCH ₂ CH ₂ COOH	178.19	10,696			116			sl s aq; s alc
b74	2-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 330			44	317	150	
b75	3-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			40	307	150	s alc, bz, eth
b76	4-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			71	315	150	s alc, bz, eth
b77	Benzyl acetate	CH ₃ COOCH ₂ C ₆ H ₅	150.18	6, 435	1.0515^{25}	1.5232^{20}	-51.5	215.5	102	sl s aq; misc alc,
										eth
b78	Benzyl alcohol	C ₆ H ₅ CH ₂ OH	108.13	6, 428	1.041325	1.5371^{25}	-15.3	205.45	100	0.08 aq; misc alc,
										eth
b79	Benzylamine	C ₆ H ₅ CH ₂ NH ₂	107.16	12, 1013	0.981_4^{19}	1.5424^{20}	10	185	60	misc aq, alc, eth
b80	2-Benzylaminoethanol	C ₆ H ₅ CH ₂ NHCH ₂ CH ₂ OH	151.21	12, 1040	1.065	1.5435^{20}		156 ^{12mm}	>112	
b81	(3-Benzylamino)-	C ₆ H ₅ CH ₂ NHCH ₂ CH ₂ CN	160.22			1.5308^{20}				
	propionitrile									

Benzoresorcinol, d386 2-Benzothiazolethiol, m17 Benzotrichloride, t248

Benzotrifluoride, t300 Benzoylamide, b4 Benzoylbenzene, b53

Benzoyl peroxide, d54 1,2-Benzphenanthrene, b6 Benzylaniline, p92



b60

b55

b56

b57

b61

Н b62

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b82 b83	N-Benzylbenzamide Benzyl benzoate	C ₆ H ₅ CONHCH ₂ C ₆ H ₅ C ₆ H ₅ COOCH ₂ C ₆ H ₅	211.26 212.25	9, 121	1.118425	1.5681 ²¹	106 19.4	323.5	147	i aq; misc alc, chl,
b84	2-Benzylbenzoic acid	C ₆ H ₅ CH ₂ C ₆ H ₄ COOH	212.24	92, 471			110–113			eth sl s aq; s alc, bz, chl, eth
b85	Benzyl bromide	C ₆ H ₅ CH ₂ Br	171.04	5, 306	1.438_0^{22}	1.5752^{20}	-3.9	198–199	86	sl d aq
b86	Benzyl- <i>tert</i> -butanol	C ₆ H ₅ CH ₂ CH ₂ - C(CH ₃) ₂ OH	164.25	6, 548		1.5090^{20}	33	144 ^{85mm}	>112	
b87	Benzyl butyl- 1,2-phthalate	C ₆ H ₅ CH ₂ OOCC ₆ H ₄ - COOC ₄ H ₀	312.37		1.119_{25}^{25}				218	
b88	Benzyl carbamate	C ₆ H ₅ CH ₂ OCONH ₂	151.17	6, 437			87–89	220 d		i aq; v s alc; sl s eth
b89	Benzyl chloride	C ₆ H ₅ CH ₂ Cl	126.59	5, 292	1.0993^{20}	1.5391^{20}	-43 to	179	73	i aq; misc alc, chl,
							-48			eth
b90	Benzyl chloroformate	C ₆ H ₅ CH ₂ OC(O)Cl	170.60	6, 437	1.195	1.5190^{20}		103 ^{20mm}	91	d aq; s eth
b91	Benzyl chlorothiol formate	C ₆ H ₅ CH ₂ S(COCl)	186.5		1.237 ₄ ³⁰	1.5711 ³⁰		80 ^{0.13mm}	118	
b92	S-Benzyl-L-cysteine	C ₆ H ₅ CH ₂ SCH ₂ - CH(NH ₂)COOH	211.28	6, 465			214 d			
b93	Benzyl diethyl phosphite	$C_6H_5CH_2P(O)(OC_2H_5)_2$	228.23		1.076	1.4930^{20}		110 ^{2mm}	>112	
b94	Benzyldimethyl- stearylammonium chloride	C ₆ H ₅ CH ₂ N[(CH ₂) ₁₇ - CH ₃](CH ₃) ₂ Cl·H ₂ O	442.18	12 ³ , 2212			67–69			
b95	Benzyl ethyl ether	C ₆ H ₅ CH ₂ OC ₂ H ₅	136.20		0.9478^{20}	1.4958^{20}		185.0		i aq; misc alc, eth
b96	N-Benzylformamide	C ₆ H ₅ CH ₂ NHCHO	135.17	12, 1043			60-61			
b97	Benzyl formate	C ₆ H ₅ CH ₂ OOCH	136.15		1.081_4^{20}			203		i aq; s alc; misc
b98	O-Benzylhydroxyl-	C ₆ H ₅ CH ₂ ONH ₂	123.16	6, 440				119 ^{30mm}		eth
	uninic .									

b99	Benzylidenemalono- nitrile	$C_6H_5CH=C(CN)_2$	154.17	9, 895			83–85			
b100	N-Benzylidenemethyl-	C ₆ H ₅ CH=NCH ₃	119.17	7, 213	0.967	1.5526 ²⁰		80 ^{18mm}	>112	
b101	3-Benzylidene- phthalide		222.24	17, 376			102			
b102	2-Benzyl-2-imid- azoline HCl		196.68				174			v s aq, alc; s chl; v sl s eth, EtAc
b103	Benzylmethylamine	C ₆ H ₅ CH ₂ NHCH ₃	138.23	12, 1019	0.939	1.5224^{20}		184.189	77	
b104	3-(N-Benzyl-N- methylamino)-1,2- propanediol	C ₆ H ₅ CH ₂ N(CH ₃)- CH ₂ CH(OH)CH ₂ OH	195.26		1.084	1.5341 ²⁰		206 ^{30mm}	>112	
b105	Benzyl methyl sulfide	C ₆ H ₅ CH ₂ SCH ₃	138.23	6, 453	1.015	1.5620^{20}		195-198	73	
b106	3-Benzyloxyaniline	C ₆ H ₅ CH ₂ OC ₆ H ₄ NH ₂	199.25	13, 404			63-67			
b107	3-Benzyloxybenz- aldehyde	C ₆ H ₅ CH ₂ OC ₆ H ₄ CHO	212.25	8,73			56–58			
b108	4-Benzyloxybenz- aldehyde	C ₆ H ₅ CH ₂ OC ₆ H ₄ CHO	212.25	8,73			73–74			

Benzyl cyanide, p80 Benzyl disulfide, d57 N-Benzylethanolamine, b80 Benzyl ether, d58 Benzylideneacetone, p96 Benzylideneacetophenone, d686 Benzyl mercaptan, p128 Benzyl methyl ketone, p144 Benzyloxyamine, b98

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b109	4-Benzyloxybenzyl alcohol	C ₆ H ₅ CH ₂ OC ₆ H ₄ CH ₂ OH	214.26				86–87			
b110 b111	2-Benzyloxyethanol 4-Benzyloxy-3-meth-	C ₆ H ₅ CH ₂ OCH ₂ CH ₂ OH C ₆ H ₅ CH ₂ OC ₆ H ₃ -	152.19 242.27		1.0720		63–65	255.9	129	0.4 aq
b112	oxybenzaldehyde 4'-Benzyloxypropio- phenone	(OCH ₃)CHO C ₆ H ₅ CH ₂ OC ₆ H ₄ COC ₂ H ₅	240.30				100–102			
b113 b114	Benzyl phenyl sulfide 1-Benzylpiperazine	C ₆ H ₅ CH ₂ SC ₆ H ₅	200.30 176.26	6, 454	1.014	1.5467 ²⁰	43	197 ^{27mm}	>112	i aq; sl s alc; s eth
b115	4-Benzylpiperidine		175.28	20, 296	0.997	1.5379^{20}	7	279	>112	s aq, alc, eth
b116 b117	1-Benzyl-4-piperidone 2-Benzylpyridine	$C_6H_5CH_2(C_5H_4N)$	189.26 169.23	20, 425	1.021 1.054	$1.5399^{20} 1.5785^{20}$	10	134 ^{7mm} 276	>112 125	i aq; v s alc, eth
b118 b119	4-Benzylpyridine 1-Benzyl-2-pyrroli- dinone	$C_6H_5CH_2(C_5H_4N)$	169.23 175.23	20, 426	$ \begin{array}{c} 1.061_0^{20} \\ 1.095 \end{array} $	$1.5818^{20} 1.5525^{20}$		287	115 >112	s alc; v s eth
b120	(Benzylthio)acetic	C ₆ H ₅ CH ₂ SCH ₂ COOH	182.24				59–63			
b121 b122	Benzyl thiocyanate Benzyltributyl- ammonium chloride	C ₆ H ₅ CH ₂ SCN C ₆ H ₅ CH ₂ N(C ₄ H ₉) ⁺ ₃ Cl ⁻	149.22 312.94	6, 460			43 155 d	235		i aq; s alc; v s eth
b123	Benzyltrichlorosilane	C ₆ H ₅ CH ₂ SiCl ₃	225.57		1.288420	1.526^{20}		140- 142 ^{100mm}		
b124	Benzyltriethoxysilane	$C_6H_5CH_2Si(OC_2H_5)_3$	254.40		0.986_4^{20}			170– 175 ^{70mm}		
b125	Benzyltriethyl- ammonium chloride	$C_6H_5CH_2N(C_2H_5)_3^+Cl^-$	227.78				185 d	173		
b126	Benzyltrimethyl- ammonium chloride	$C_6H_5CH_2N(CH_3)_3^+C1^-$	185.70	12, 1020						

b127	Benzyltrimethyl- silane	$C_6H_5CH_2Si(CH_3)_3$	164.32		0.8933^{20}	1.4941 ²⁰		190–191		
b128	Betaine	$(CH_3)_3$ $\overset{+}{N}CH_2COO^-$	117.15	4, 347			d>310			160 aq; 55 MeOH;
b129	Bicyclo[2.2.1]hepta- 2,5-diene		92.14		0.909^{20}	1.4707 ²⁰	-20	89	-21	6 alc i aq; s PE
b130	Bicyclo[2.2.1]-2- heptene		94.16				46	96	-15	s eth
b131	Bicyclo[2.2.1]-5- heptene-2-carbal-		122.16		1.018	1.4883 ²⁰		67- 70 ^{12mm}	51	
	dehyde									

Benzylphenol, h113 BES, b180 Betahistine, m121 *o,o*-Bibenzoic acid, b137 Bibenzyl, d666 Bicine, b182

b130

Bicyclo[4.4.0]decane, d1, d2

HC=0

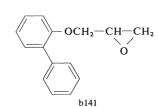
TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b132	Bicyclo[2.2.2]oct-7- ene-2,3,5,6-tetracar- boxylic-2,3,5,6-di- anhydride		248.19				>300			
b133	Biguanide	$H_2NC(=NH)NHC-$ $(=NH)NH_2$	101.11	3,93			130	d 142		s aq, alc; i bz, eth
b134	Biphenyl	$C_6H_5-C_6H_5$	154.20	5, 578	0.9939^{70}	1.58877	68.8	255.0		i aq; s alc, eth
b135	4-Biphenylcarboxylic acid	C ₆ H ₅ C ₆ H ₄ COOH	198.22	9, 671			226	subl		i aq; v s alc, eth; s bz
b136	(1,1'-Biphenyl)-4,4'- diamine	$H_2NC_6H_4C_6H_4NH_2$	184.23	13, 214			128	400 ^{740mm}		0.04 aq; s alc; 2 eth
b137	(1,1'-Biphenyl)-2,2'- dicarboxylic acid	HOOCC ₆ H ₄ C ₆ H ₄ COOH	242.23	9,922			228–229			0.06 aq; s org solv
b138	4-Biphenylmethanol	C ₆ H ₅ C ₆ H ₄ CH ₂ OH	184.24	$6^2,636$			101			
b139	4-Biphenylsulfonic acid	$C_6H_5C_6H_4SO_3H$	234.26				138			
b140	2-(4-Biphenylyl)- 5-(4- <i>tert</i> - butylphenyl)- 1,3.4-oxadiazole		354.46				138			
b141	o-Biphenylyl glycidyl ether		226.28				30–32	120 ^{0.1mm}		
b142	2-(4-Biphenylyl)-5- phenyloxazole		197.36				118			
b143	2,2'-Bipyridinium chlorochromate	$C_5H_4N-C_5H_4NH^+CrClO_3^-$	292.64							
b144	2,2-Bis[<i>p</i> -(allyloxy)-phenyl]propane	H ₂ C=CHCH ₂ OC ₆ H ₄ C- (CH ₃) ₂ C ₆ H ₄ OCH ₂ - CH=CH ₂	308.42		1.022	1.5636 ²⁰			>112	

b145	N,N'-Bis(3-amino- propyl)-ethylenedi- amine	H ₂ N(CH ₂) ₃ NHCH ₂ CH ₂ - NH(CH ₂) ₃ NH ₂	174.29					118 ^{0.2mm}	
b146	N,N'-Bis(3-amino-		200.33	23 ² , 12	0.973	1.5015^{20}	15	152 ^{2mm}	
b147	propyl)piperazine <i>N,N'</i> -Bis(3-amino-	H ₂ N(CH ₂) ₃ NHCH ₂ CH ₂ -	188.32					98–103 ^{1mm}	
	propyl)-1,3- propanediamine	CH ₂ NH(CH ₂) ₃ NH ₂							
b148	2,5-Bis(4-biphenylyl)-		373.46				240		
	oxazole								

Bicyclo[4.3.0]nonane, h46 Biphenol, d387 Biphenylamines, a134, a135 3-(*o*-Biphenylyloxy)-1,2-epoxypropane, b142 2,2'-Bipyridine, d705 Bis(4-aminophenyl)ether, o61

1,3-Bis(aminomethyl)cyclohexane, c314 1,2-Bis(benzylamino)ethane, d59



b148

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b149	Bis(2-bromoethyl)	BrCH ₂ CH ₂ OCH ₂ CH ₂ Br	231.92					103-		
b150	ether 1,3-Bis(bromoethyl)- tetramethyldi-	[BrCH ₂ Si(CH ₃) ₂] ₂ O	320.17		1.3918420	1.4719 ²⁰		107 ²⁰ 103– 104 ^{15mm}		
b151	siloxane Bis(2-butoxyethyl) ether	(C ₄ H ₉ OCH ₂ CH ₂) ₂ O	218.33		0.885320	1.4233 ²⁰	-60.2	254.6	47	0.3 aq; misc alc, eth, ketones, esters, CCl ₄
b152	2,5-Bis(5- <i>tert</i> -butyl- 2'-benzoxazolyl)- thiophene		430.57				201			CSICIS, CCI ₄
b153	Bis(sec-butyl) disulfide	[CH ₃ CH ₂ CH(CH ₃)] ₂ S ₂	178.36	1 ³ , 1549	0.957	1.4920 ²⁰		164 ^{739mm}	>112	
b154	Bis(tert-butyl) disulfide	(CH ₃) ₃ CSSC(CH ₃) ₃	178.36	1, 379	0.909	1.4930 ²⁰		204	79	
b155	Bis(carboxymethyl) trithiocarbonate	HOOCCH ₂ SC(=S)- SCH ₂ COOH	226.29	3, 252			172–175			
b156	1,2-Bis(2-chloro- ethoxy)ethane	(CICH ₂ CH ₂ OCH ₂ —) ₂	187.07		1.197_4^{20}	1.4617		108 ^{8mm}		
b157	Bis(2-chloroethoxy)- methylsilane	H(CH ₃)Si- (OCH ₂ CH ₂ Cl) ₂	203.1		1.1643420	1.4431 ²⁰		95–97 ^{18mm}		
b158	Bis(2-chloroethyl) ether	CICH ₂ CH ₂ OCH ₂ CH ₂ CI	143.01	1 ² , 335	1.219220	1.4575 ²⁰	-51.7	178.8	55	i aq; s most org solv
b159	Bis(2-chloroethyl)- N-methylamine	CH ₃ N(CH ₂ CH ₂ Cl) ₂	156.07		1.118425		-60	75 ^{10mm}		v sl s aq; misc most org solv
b160	Bis(chloromethyl)- dimethylsilane	(CH ₃) ₂ Si(CH ₂ Cl) ₂	157.12	4 ³ , 1845	1.075 ²⁰	1.4600 ²⁰		160		

b161	Bis(2-chloro-1- methyl)ethyl ether	CICH ₂ CH(CH ₃)OCH- (CH ₃)CH ₂ Cl	171.07		1.1122_{20}^{20}			187.3	85	
b162	Bis(4-chloro- phenoxy)- acetic acid	(CIC ₆ H ₄ O) ₂ CHCOOH	313.14				142			
b163	2,2-Bis(<i>p</i> -chloro- phenyl)-1,1-di- chloroethane	(ClC ₆ H ₄) ₂ CHCHCl ₂	320.05				111			
b164	1,1-Bis(4'-chloro- phenyl)ethanol	(CIC ₆ H ₄) ₂ C(OH)CH ₃	267.16	6 ³ , 3396			69			v sl s aq; s org solv
b165	Bis(4-chlorophenyl) sulfone	ClC ₆ H ₄ SO ₂ C ₆ H ₄ Cl	287.16	6, 327				250 ^{10mm}		
b166	Bis(4-chlorophenyl) sulfoxide	ClC ₆ H ₄ S(O)C ₆ H ₄ Cl	271.17	6 ¹ , 149			144			
b167	1,1-Bis(<i>p</i> -chloro- phenyl)-2,2,2-tri- chloroethane	(CIC ₆ H ₄) ₂ CHCCl ₃	354.49				109			i aq; 58 acet; 78 bz; 45 CCl ₄ ; v s pyr, diox
b168	1,3-Bis(dichloro- methyl)tetramethyl- disiloxane	[Cl ₂ CH(CH ₃) ₂ Si] ₂ O	300.16		1.2213420	1.4660 ²⁰		149 ^{40mm}		
b169	N,N-Bis(2,2-dieth- oxyethyl)- methylamine	[(C ₂ H ₅ O) ₂ CHCH ₂] ₂ - NCH ₃	263.38	4, 311	0.945	1.4259 ²⁰		222 ^{244mm}	60	

Bis(3-*tert*-butyl-4-hydroxy-5-methylphenyl) sulfide, t144

Bis(2-cyanoethyl) ether, o63

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b170	4,4'-Bis(diethyl- amino)benzo- phenone	$[(C_2H_5)_2NC_6H_4]_2C = O$	324.47	14, 98			95			
b171	4,4'-Bis(dimethyl- amino)benzo- phenone	[(CH3)2)NC6H4]2C(=O)	268.36	14, 89			172–176	d 360		i aq; s alc, warm bz
b172	Bis(dimethylamino)- dimethylsilane	[(CH ₃) ₂ N] ₂ Si(CH ₃) ₂	146.3		0.810 ²²	1.432 ²²	-98	128–129		
b173	1,3-Bis(dimethyl- amino)-2-propanol	[(CH ₃) ₂ NCH ₂] ₂ CHOH	146.23	4, 290	0.897	1.4422 ²⁰			>112	
b174	Bis(dimethylthio- carbamyl) disulfide	[(CH3)2NC(=S)S-]2	240.43	4, 76	1.29		155–156			s alc, eth; sl s bz, acet; i aq
b175	1,4-Bis(2,3-epoxy- propoxy)butane	H ₂ C CHCH ₂ - OCH ₂ CH ₂ -],	202.25		1.049	1.4535 ²⁰		160 ^{11mm}	>112	
b176	Bis(2-ethoxyethyl) ether	$(C_2H_5OCH_2CH_2)_2O$	162.23	1 ² , 519	0.907_4^{20}	1.4110^{20}	-44.3	188.4	54	v s aq, alc, org solv
b177	Bis(2-ethylhexyl) decanedioate	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ OOC(CH ₂) ₈ COOCH ₂ - CH(C ₂ H ₅)(CH ₂) ₃ CH ₃	426.66		1.911925	1.4496 ²⁵				
b178	Bis(2-ethylhexyl) hydrogen phosphate	[CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ O] ₂ P(O)OH	322.43	1 ⁴ , 1786	0.965	1.4450 ²⁰	-60	209 ^{10mm}		
b179	Bis(2-ethylhexyl) o-phthalate	[CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ OOC] ₂ C ₆ H ₄	390.57		0.984320	1.4859 ²⁰	-50	384	207	0.01 aq
b180	N,N-Bis(2-hydroxy- ethyl)-2-amino- ethanesulfonic acid	(HOC ₂ H ₅) ₂ - NCH ₂ CH ₂ SO ₃ H	213.25				152–154			
b181	Bis(2-hydroxyethyl) ether	HOCH ₂ CH ₂ OCH ₂ CH ₂ OH	106.12	1, 468	1.118_{20}^{20}	1.4460 ²⁰	-10.45	245	143	misc aq, alc, acet, eth

b182	N,N-Bis(2-hydroxy-	$(HOCH_2CH_2)_2NCH_2COOH$	163.17				192 sl d			sl s aq
b183	ethyl)glycine Bis(2-hydroxyethyl)- iminotris(hydroxy- methyl)methane	(HOCH ₂ CH ₂) ₂ - NC(CH ₂ OH) ₃	209.24				104			
b184	2,2-Bis(hydroxy- methyl)propionic	(HOCH ₂) ₂ C(CH ₃)COOH	134.13	3, 401			189–191			
b185	4,8-Bis(hydroxy- methyl)tricyclo- [5.2.0 ^{2,6}]decane		196.29			1.5280 ²⁰			>112	
b186	Bis(2-mercaptoethyl) ether	(HSCH ₂ CH ₂) ₂ O	138.25		1.114		-80	217		
b187	Bis(2-mercaptoethyl) sulfide	$(HSCH_2CH_2)_2S$	154.32		1.183	1.598220		136 ^{10mm}	90	
b188	1,4-Bis(methane- sulfonoxy)butane	(CH ₃ SO ₂ OCH ₂ CH ₂ —) ₂	246.30				115–117			sl hyd aq; 0.1 alc; 1.4 acet
b189	1,2-Bis(methoxy- ethoxy)ethane	(CH ₃ OCH ₂ CH ₂ OCH ₂ —) ₂	178.23		0.990_4^{20}	1.4224 ²⁰	-45	216	110	misc aq
b190	Bis[2,(2-methoxyeth- oxy)ethyl] ether	(CH ₃ OCH ₂ CH ₂ OCH ₂ - CH ₂ —) ₂ O	222.28	1 ³ , 2107	1.0087420	1.4330^{20}	-27	275.3	140	s aq
b191	Bis(2-methoxyethyl) ether	(CH ₃ OCH ₂ CH ₂ —) ₂ O	134.18		0.9440 ²⁵	1.4043 ²⁵	-68	162	70	misc aq

Bis(2-ethylhexyl) sebacate, b177 Bis(2-hydroxyethyl) sulfide, t149 2,2-Bis(hydroxymethyl)-2,2',2"-nitrilotriethanol, b183

Bis(4-hydroxyphenyl) sulfide, t150

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b192	Bis(2-methylallyl) carbonate	[H2C=C(CH3)CH2O]2-C(=O)	170.21		0.94320	1.4371		202	72	
b193	Bis(4-nitrophenyl) carbonate	$(O_2NC_6H_4O)_2C(=O)$	304.21	6 ¹ , 120			141			
b194	Bis(3-nitrophenyl) disulfide	O ₂ NC ₆ H ₄ SSC ₆ H ₄ NO ₂	308.22	6, 339			83			i aq; s alc, eth
b195	Bis(4-nitrophenyl) disulfide	O ₂ NC ₆ H ₄ SSC ₆ H ₄ NO ₂	308.33	6, 340			181			sl s alc
b196	Bis(octadecyl)penta- erythritol diphosphite	[C ₁₈ H ₃₇ OP(OCH ₂) ₂] ₂	721.01		0.925	1.457	40		261	
b197	Bis(pentabromo- phenyl) ether	C ₆ Br ₅ OC ₆ Br ₅	969.22	6 ¹ , 108			>300			
b198	1,4-Bis(5-phenyloxa- zol-2-yl)benzene		364.40				244			
b199	Bis(p-tolyl) disulfide	CH ₃ C ₆ H ₄ SSC ₆ H ₄ CH ₃	246.39	6, 425			43–46			i aq; s alc; v s eth
b200	Bis(<i>p</i> -tolyl) sulfoxide	CH ₃ C ₆ H ₄ S(O)C ₆ H ₄ CH ₃	230.33	6, 419			94–96			v s alc, bz, chl, eth
b201	Bis(tributyltin) oxide	$(C_4H_9)_3SnOSn(C_4H_9)_3$	596.08		1.170	1.4864 ²⁰		180 ^{2mm}	>112	
b202	1,4-Bis(trichloro- methyl)benzene	Cl ₃ CC ₆ H ₄ CCl ₃	312.84	5, 385			108–110			i aq; 26 acet; 38 bz; 22 CCl ₄ ; 33 eth; 3 MeOH
b203	Bis(2,4,5-trichloro- phenyl) disulfide	Cl ₃ C ₆ H ₄ SSC ₆ H ₄ Cl ₃	425.01				140–144			0, 5 112011
b204	1,2-Bis(trichloro-silyl)ethane	Cl ₃ SiCH ₂ CH ₂ SiCl ₃	296.64		1.483420	1.473 ²⁰	24.5	201–202		
b205	3,5-Bis(trifluoro- methyl)aniline	$(F_3C)_2C_6H_3NH_2$	229.13		1.467	1.4335 ²⁰		85 ^{15mm}	83	

b206	1,3-Bis(trifluoro- methyl)benzene	F ₃ CC ₆ H ₄ CF ₃	214.0	1.3790 ²⁵	1.3916 ²⁵		116	
b207	N,O-Bis(trimethyl-silyl)acetamide	CH ₃ C=N-Si(CH ₃) ₃ O-Si(CH ₃) ₃	203.43	0.832420	1.4170 ²⁰		73 ^{35mm}	11
b208	Bis(trimethylsilyl)- acetylene	(CH ₃) ₃ SiC≡CSi(CH ₃) ₃	170.41	0.770_4^{20}	1.413 ²⁰		137	2
b209	Bis(trimethylsilyl)- formamide	HC=NSi(CH ₃) ₃ O-Si(CH ₃) ₃	189.41	0.885	1.4381 ²⁰		54– 55 ^{13mm}	
b210	N,O-Bis(trimethyl-silyl)hydroxyl-amine	(CH ₃) ₃ SiONHSi(CH ₃) ₃	177.40	0.830	1.4112 ²⁰		78- 80 ^{100mm}	28
b211	1,2-Bis(trimethyl-silyloxy)ethane	(CH ₃) ₃ SiOCH ₂ CH ₂ - OSi(CH ₃) ₃	206.43	0.842	1.4034^{20}		165–166	46
b212	N,O-Bis(trimethyl-silyl)trifluoroacet-amide	$CF_3C[=NSi(CH_3)_3]-OSi(CH_3)_3$	257.40	0.969	1.3939 ²⁰	-10	50 ^{14mm}	23
b213	Bis(triphenyl- phosphine)di- carbonylnickel	$[(C_6H_5)_3P]_2Ni(CO)_2$	639.32			209		

Bis(phenylmethyl) disulfide, d57

"Bis-tris," b183

"Bis-tris" propane, b214

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b214	1,3-Bis[tris(hydroxy- methyl)methyl- amino]propane	CH ₂ [CH ₂ NHC (CH ₂ OH) ₃] ₂	282.34	4 ³ , 859			170			
b215	Biuret	H ₂ NCONHCONH ₂	103.08	3, 70	1.467_4^{-5}		110	d 190		v s alc; 2 aq
b216	1-Borneol		154.25	6, 72	1.011_4^{20}		204	212	65	i aq; 176 alc; s eth, bz, PE
b217	1-Bornyl acetate		196.29	6, 82	0.982	1.4626	27	224	84	sl s aq; s alc, eth
b218	N-Bromoacetamide	CH₃CONBrH	137.97	2, 181			102-105			sl s aq; v s eth
b219	<i>p</i> -Bromoacetanilide	BrC ₆ H ₄ NHCOCH ₃	214.07	12, 642	1.717		168			i aq; s bz, chl, EtAc
b220	Bromoacetic acid	BrCH₂COOH	138.95	2, 213	1.934_4^{50}	1.4804^{50}	50	208		v s aq, alc, eth
b221	α-Bromoaceto-	C ₆ H ₅ COCH ₂ Br	199.05	7, 283	1.647_4^{20}		50	135 ^{18mm}		i aq; v s alc, bz,
	phenone									chl, eth
b222	p-Bromoaceto-	BrC ₆ H ₄ COCH ₃	199.05	7, 283	1.647		54	255		s alc, bz, eth,
	phenone									HOAc
b223	Bromoacetyl bromide	BrCH ₂ COBr	201.86	2, 215	2.317_{22}^{22}	1.5480^{20}		150	none	d aq, alc
b224	Bromoacetyl chloride	BrCH ₂ COCl	157.40	2, 215	1.908	1.4960^{20}		128	none	d aq, alc
b225	2-Bromoaniline	BrC ₆ H ₄ NH ₂	172.03	12,631	1.578_4^{20}	1.6113^{20}	31	229		i aq; s alc, eth
b226	3-Bromoaniline	BrC ₆ H ₄ NH ₂	172.03	12,633	1.580_4^{20}	1.6250^{20}	16.8	251	>112	sl s aq; s alc, eth
b227	4-Bromoaniline	BrC ₆ H ₄ NH ₂	172.03	12,636	1.4970_4^{100}		66.3			i aq; v s alc, eth
b228	3-Bromobenzaldehyde	BrC ₆ H ₄ CHO	185.03	7, 238	1.587	1.5935^{20}		230	96	i aq; v s alc, eth
b229	Bromobenzene	C ₆ H ₅ Br	157.02	5, 206	1.49524	1.5580 ²⁰	-30.72	156.2	51	0.044 aq; 10.4 alc; misc bz, chl, PE; 71.6 eth
b230	Bromobenzene-d ₅	C ₆ D ₅ Br	162.06					53 ^{23mm}	65	
b231	4-Bromobenzene-	BrC ₆ H ₄ SO ₂ Cl	255.52	11,57			74.5	153 ^{15mm}	"	i aq; d alc; v s eth
	sulfonyl chloride	0 4 2 -		,						1, ,
b232	4-Bromobenzo-	BrC ₆ H ₄ COC ₆ H ₅	261.12	7,422				82	350	i alc; sl s bz, eth
	phenone									
	1	ı	1	1	1	1	1	1		1

b233	2-Bromobenzotri-	BrC ₆ H ₄ CF ₃	225.01		1.65220	1.4817^{20}		168	51	
	fluoride									
b234	3-Bromobenzotri-	BrC ₆ H ₄ CF ₃	225.01		1.613	1.4749^{20}		152	43	
	fluoride									
b235	2-Bromobenzyl	BrC ₆ H ₄ CH ₂ OH	187.04	6, 445			82			s hot aq; v s alc,
	alcohol									eth
b236	2-Bromobenzyl	BrC ₆ H ₄ CH ₂ Br	249.94	5, 308		1.6193^{20}	31	129 ^{19mm}		d hot aq; s alc, eth
	bromide									
b237	4-Bromobiphenyl	BrC ₆ H ₄ C ₆ H ₅	233.11	5, 580	9.9327_4^{25}		87	310		i aq; s alc, bz, eth
b238	1-Bromobutane	CH ₃ CH ₂ CH ₂ CH ₂ Br	137.02	1, 119	1.2686_4^{25}	1.4374^{25}	-112.4	101.6	23	i aq; s alc, bz, eth
b239	2-Bromobutane	CH ₃ CH ₂ CHBrCH ₃	137.03	1, 119	1.2530_4^{25}	1.4360^{20}	-112.4	21		<0.1 aq; v s alc,
										eth
b240	1-Bromo-2-butene	CH ₃ CH=CHCH ₂ Br	135.01	1, 205	1.312	1.4765^{20}		99	11	
b241	2-Bromo-2-butene	$CH_3CH = C(Br)CH_3$	135.01	1, 205	1.328	1.4613^{20}		90 ^{740mm}	<1	
b242	4-Bromo-1-butene	BrCH ₂ CH ₂ CH=CH ₂	135.01	1 ¹ , 84	1.3230_4^{20}	1.4608^{30}		100	<1	i aq; s alc, eth

2-Bornanone, c3 Bromal, t201 Bromoacetaldehyde diethyl acetal, b267 Bromoanisoles, b301, b302, b303 *p*-Bromobenzenethiol, b354 4-Bromobenzyl cyanide, b329

*exo-*2-Bromobicyclo[2.2.1]heptane, b318 Bromobutanedioic acid, b350

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b243	4-Bromobutyl phenyl ether	C ₆ H ₅ OCH ₂ CH ₂ CH ₂ CH ₂ Br	229.12	62,82			41–42	153- 156 ^{18mm}		
b244 b245	2-Bromobutyric acid endo-3-Bromo-D-camphor	CH ₃ CH ₂ CH(Br)COOH	167.01 231.14	2, 281 7 ² , 101	1.5669 ²⁰ 1.449	1.4720 ²⁰	-4 76–78	103 ^{10mm} 244	>112	6.7 aq; s alc, eth i aq; 15 alc; 200 chl; 62 eth
b246	α-Bromo- <i>p</i> -chloro- acetophenone	ClC ₆ H ₄ COCH ₂ Br	233.50	7, 285			96.5			0111, 02 0111
b247	2-Bromochloroben- zene	BrC ₆ H ₄ Cl	191.46	5, 209	1.6382425	1.5789 ²⁵		204	79	i aq; v s bz
b248	3-Bromochloroben- zene	BrC ₆ H ₄ Cl	191.46	5, 209	1.6302_4^{20}	1.5771 ²⁰	-21	196	80	i aq; v s alc, eth
b249	4-Bromochloroben- zene	BrC ₆ H ₄ Cl	191.46	5, 209	1.576471	1.5531 ⁷⁰	64.5	196		0.1 aq; misc MeOH, eth
b250	3-Bromo-4-chloro- benzotrifluoride	Br(Cl)C ₆ H ₃ CF ₃	259.47		1.743 ²⁵	1.4973 ²⁵	-22	191–192		112011, 0111
b251	1-Bromo-4-chloro- butane	ClCH ₂ CH ₂ CH ₂ CH ₂ Br	171.47	5 ³ , 294	1.488	1.4875 ²⁰		82 ^{30mm}	60	i aq; s alc, chl, eth
b252	4-Bromo-6-chloro- <i>o</i> -cresol	Br(Cl)C ₆ H ₂ (OH)CH ₃	221.49	6, 360			47			
b253	Bromochlorodifluoro- methane	Br(Cl)CF ₂	165.4		1.83 ²¹		-160.5	-4.01		
b254	1-Bromo-2-chloro- ethane	ClCH ₂ CH ₂ Br	143.43	1, 89	1.7392_4^{20}	1.4917 ²⁰	-18.4	106.6	none	0.7 aq; misc org solv
b255	7-Bromo-5-chloro-8- hydroxyguinoline		258.51	211, 222			177–179			
b256	Bromochloromethane	CICH ₂ Br	129.39	1,67	1.923425	1.480 ²⁵	-88	67.8	none	0.9 aq; misc MeOH, eth

b257	1-Bromo-3-chloro- propane	CICH ₂ CH ₂ CH ₂ Br	157.44	1, 109	1.472	1.486^{20}	<-50	143.5	none	0.1 aq; misc org
b258	2-Bromo-2-chloro- 1,1,1-trifluoro-	HC(Br)ClCF ₃	197.4		1.8636 ²⁵	1.3738 ²⁵		50		
	ethane									
b259	α-Bromocinnamal-	$C_6H_5CH = C(Br)CHO$	211.06	7, 358			66-68			
	dehyde									
b260	Bromocycloheptane	BrC ₇ H ₁₃	177.09	5, 29	1.2887_4^{22}	1.5052^{20}		72 ^{10mm}	68	i aq; v s chl, eth
b261	Bromocyclohexane	BrC ₆ H ₁₁	163.06	5, 24	1.3264_4^{15}	1.4956^{15}		165.8	62	0.1 aq; 10 MeOH;
										71 eth
b262	3-Bromocyclohexene		161.04	$5^2, 40$	1.3890_4^{20}	1.5292^{20}		64-65 ^{15mm}		
b263	Bromocyclopentane	BrC ₅ H ₉	149.04	5, 19	1.3900_4^{20}	1.4881^{20}		137–139	35	
b264	Bromocyclopropane	BrC ₃ H ₅	120.98			1.4605^{20}		69	2	
b265	1-Bromodecane	CH ₃ (CH ₂) ₉ Br	221.19	1 ² , 130	1.0658_4^{20}	1.4560^{20}	-30	238	94	i aq; v s chl, eth
b266	Bromodi-	HCBrCl ₂	163.83	1,67	1.980^{20}	1.4964^{20}	-55	89.2	none	sl s aq; misc org
	chloromethane									solv
b267	2-Bromo-1,1-di-	BrCH ₂ CH(OC ₂ H ₅) ₂	197.08	1,625	1.310	1.4385^{20}		67 ^{18mm}	51	s hot alc
	ethoxyethane							180 d		

2-Bromo-p-cumene, b298 β -Bromocumene, b297

4-Bromodiphenyl ether, b330

Bromoethene, b284

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b268	4-Bromo-1,2-di- methoxybenzene	BrC ₆ H ₃ (OCH ₃) ₂	217.07	6, 784	1.702	1.574320		256	109	
b269	1-Bromo-2,2-di- methoxypropane	CH ₃ C(OCH ₃) ₂ CH ₂ Br	183.05		1.355	1.4475 ²⁰		87 ^{80mm}	40	
b270	4-Bromo-2,6-di- methylphenol	BrC ₆ H ₂ (CH ₃) ₂ OH	201.07	6, 485			78			
b271	2-Bromo-4,6-di- nitroaniline	BrC ₆ H ₂ (NO ₂) ₂ NH ₂	262.02	12,761			154	subl		v s hot alc, hot acet
b272	3-Bromo-4,6-di- nitrofluorobenzene	BrC ₆ H ₂ (NO ₂) ₂ F	264.9				90–91			
b273	2-Bromo-2,2-di- phenylacetyl bromide	BrC(C ₆ H ₅) ₂ COBr	354.05	91, 283			63–65			
b274	α-Bromodiphenyl- methane	$C_6H_5CH(Br)C_6H_5$	247.14	5, 592			40	184 ^{20mm}		
b275	1-Bromododecane	CH ₃ (CH ₂) ₁₁ Br	249.24	1 ² , 133	1.038	1.4580^{20}	-9	135 ^{6mm}	110	0.1 aq; s alc, eth
b276	1-Bromo-2,3-epoxy- propane	H ₂ C—CHCH ₂ Br	136.98	17,9	1.601 ²⁰	1.4820 ²⁰	-40	134–136	56	i aq; sl s alc; s eth
b277	Bromoethane	CH ₃ CH ₂ Br	108.97	1,88	1.470815	1.427615	-118.6	38.4	none	0.91 aq
b278	2-Bromoethane- sulfonic acid, sodium salt	BrCH ₂ CH ₂ SO ₃ ⁻ Na ⁺	211.02	4,7			283– 285 d			
b279	2-Bromoethanol	BrCH ₂ CH ₂ OH	124.97	1,338	1.7629_4^{20}	1.4920^{20}		150	40	misc aq; s org solv
b280	2-Bromoethyl acetate	CH ₃ COOCH ₂ CH ₂ Br	167.01	2 ¹ , 57	1.514420	1.4547 ²⁰	-13.8	159	71	v s aq; misc alc, eth
b281	2-Bromoethylamine HBr	BrCH ₂ CH ₂ NH ₂ ·HBr	204.90	4, 134			172–174			v s aq, alc

b282	o-Bromo(ethyl)- benzene	CH ₃ CH ₂ C ₆ H ₄ Br	185.07	5, 355	1.3566_{25}^{25}	1.5603^{20}		199		0.1 aq; misc org
b283	(2-Bromoethyl)- benzene	C ₆ H ₅ CH ₂ CH ₂ Br	185.07	5, 356	1.355	1.5563 ²⁰		221	89	i aq; s bz, eth
b284	Bromoethylene	H ₂ C=CHBr	106.96	1, 188	1.493^{20}	1.4350^{20}	-139.5	15.8		i aq; misc alc, eth
b285	2-Bromoethyl ethyl ether	BrCH ₂ CH ₂ OCH ₂ CH ₃	153.02	1, 338	1.3572420	1.4450^{20}		150	21	sl s aq; misc alc, eth
b286	2-Bromoethyl phenyl ether	BrCH ₂ CH ₂ OC ₆ H ₅	201.07	6, 142			34	144 ^{40mm}	65	i aq; v s alc, eth
b287	N-(2-Bromoethyl)- phthalimide		254.09	21, 461			81–84			s hot aq; v s eth
b288	2-Bromofluoro- benzene	BrC ₆ H ₄ F	175.01		1.601	1.5337 ²⁰		156	43	
b289	3-Bromofluoro- benzene	BrC ₆ H ₄ F	175.01		1.567	1.5257 ²⁰		150	38	
b290	4-Bromofluoro- benzene	BrC ₆ H ₄ F	175.01	5, 209	1.59315	1.531015	-17.4	151–152	60	
b291	1-Bromoheptane	H(CH ₂) ₇ Br	179.11	1, 155	1.1384_4^{20}	1.4505^{20}	-58	180	60	i aq; v s alc, eth
b292	2-Bromoheptane	H(CH ₂) ₅ CH(Br)CH ₃	179.11	1, 155	1.142	1.4470^{20}		66 ^{21mm}	47	_
b293	1-Bromohexadecane	H(CH ₂) ₁₆ Br	305.35	1 ² , 138	0.9991	1.4618	17.8	336	177	i aq; misc org solv
b294	1-Bromohexane	H(CH ₂) ₆ Br	165.08	1, 144	1.1763_4^{20}	1.4475	-85	154–158	57	i aq; misc alc, eth

(Bromomethyl)benzene, b85

Bromoform, t206

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b295	DL-2-Bromohexanoic acid	CH ₃ (CH ₂) ₃ CH(Br) COOH	195.06	2, 325	1.370	1.472020		136– 138 ^{18mm}		
b296 b297	5-Bromoisatin (2-Bromoisopropyl)- benzene	C ₆ H ₅ CH(CH ₃)CH ₂ Br	226.03 199.10	21, 453 5 ¹ , 191	1.316	1.5480 ²⁰	251–253	108 ^{18mm}	91	
b298	2-Bromo-4-isopropyl- 1-methylbenzene	CH ₃ (Br)C ₆ H ₃ CH(CH ₃) ₂	213.0		1.253_{25}^{25}	1.535 ²⁵	-20	120		i aq; 50 MeOH; misc org solv
b299	Bromomaleic anhydride		176.96	17, 435	1.905	1.5400 ²⁰		215	>112	misc org sorv
b300	Bromomethane	CH₃Br	94.94	1,67	1.7320	1.423410	-84	3.56	none	0.1 aq; s alc, chl,
b301	2-Bromo-1-methoxy- benzene	BrC ₆ H ₄ OCH ₃	187.04	6, 197	1.5018425	1.5737 ²⁰	2	223	96	i aq; v s alc, eth
b302	3-Bromo-1-methoxy- benzene	BrC ₆ H ₄ OCH ₃	187.04	6, 198	1.477	1.5635 ²⁰	211	93		i aq; s alc, eth
b303	4-Bromo-1-methoxy- benzene	BrC ₆ H ₄ OCH ₃	187.04	6, 199	1.4564 ₄ ²⁰	1.5630 ²⁰	10	223	94	sl s aq; v s alc, eth
b304	4-Bromo-2-methyl-	CH ₃ (Br)C ₆ H ₃ NH ₂	186.06	12, 838			56	240		sl s aq; v s alc
b305	1-Bromo-3-methyl- butane	(CH ₃) ₂ CHCH ₂ CH ₂ Br	151.05	1, 136	1.210_4^{15}	1.4409 ²⁰	-112	119.7	32	0.02 aq; misc alc, eth
b306	(Bromomethyl)cyclo- hexane	C ₆ H ₁₁ CH ₂ Br	177.09	$5^2, 18$	1.269	1.4907 ²⁰		76–77 ^{26mm}	57	
b307	2-Bromomethyl-1,3- dioxalane		167.01	19 ² , 8	1.613	1.4817 ²⁰		80-82 ^{27mm}	62	
b308	Bromomethyl methyl ether	BrCH ₂ OCH ₃	124.97	1,582	1.531	1.4550 ²⁰		87	26	

0.06 ag; misc alc,
0.06 ag: misc alc.
eth
i aq; misc org solv
misc alc, bz, chl,
i ag; s alc, bz, eth
v s alc; s bz, eth
i aq; s chl, eth
i aq; s alc, eth

 α -Bromoisobutyrophenone, b311a

2-Bromomesitylene, b362

 α -Bromo-4-nitro-o-cresol, h155

 α -Bromo-p-nitrotoluene, n46

$$O \longrightarrow O \longrightarrow CH_2B$$

b307

b318

137

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b320	1-Bromooctane	H(CH ₂) ₈ Br	193.13	1, 160	1.108_4^{25}	1.4503 ²⁵	-55	201	78	i ag; misc alc, eth
b321	Bromopentafluoro- benzene	BrC ₆ F ₅	246.97		1.947 ²⁰	1.4490^{20}	-31	137	87	
b322	1-Bromopentane	H(CH ₂) ₅)Br	151.05	1, 131	1.2337 ₄ ¹⁵	1.4444 ²⁰	-88	129.6	31	i aq; s alc; misc eth
b323	2-Bromopentane	CH ₃ CH ₂ CH ₂ CH(Br)CH ₃	151.05	1, 131	1.2039_4^{20}	1.4403^{20}		117	20	
b324	9-Bromophenanthrene		257.14	5, 671	1.409_4^{101}		54-58	190 ^{2mm}		i aq; s alc, eth
b325	2-Bromophenol	BrC ₆ H ₄ OH	173.01	6, 197	1.492	1.5892^{20}	6	194	42	s aq; misc chl, eth
b326	4-Bromophenol	BrC ₆ H ₄ OH	173.01	6, 198	1.587580		68	238		14 aq; v s alc, chl
b327	2-Bromo-2-phenyl- acetic acid	C ₆ H ₅ CH(Br)COOH	215.05	9, 451			83			
b328	<i>p</i> -Bromophenylacetic acid	BrC ₆ H ₄ CH ₂ COOH	215.05	9, 451			119			sl s aq; v s alc, eth
b329	<i>p</i> -Bromophenylaceto- nitrile	BrC ₆ H ₄ CH ₂ CN	196.05	9, 451			47–49			i aq; sl s alc; v s bz
b330	4-Bromophenyl phenyl ether	BrC ₆ H ₄ OC ₆ H ₅	249.11	6 ¹ , 105	1.423	1.6070^{20}	18	305	>112	
b331	1-Bromo-3-phenyl- propane	C ₆ H ₅ CH ₂ CH ₂ CH ₂ Br	199.10	5, 391	1.310	1.5450^{20}		220	101	
b332	1-Bromopropane	CH ₃ CH ₂ CH ₂ Br	123.00	1, 108	1.359715	1.4370^{15}	-110.1	71.0	25	0.23 aq ³⁰ ; misc alc
b333	2-Bromopropane	CH ₃ CH(Br)CH ₃	123.00	1, 108	1.322215	1.428515	-89.0	59.5	19	0.3 aq ¹⁸ ; misc alc, bz, chl, eth
b334	3-Bromo-1-propanol	BrCH ₂ CH ₂ CH ₂ OH	139.00	1,356	1.5374_4^{20}	1.4858^{20}		62 ^{5mm}		s ag; misc alc, eth
b335	1-Bromo-1-propene	CH ₃ CH=CHBr	120.98	1,200	1.4133_{4}^{20}	1.4538^{20}	-116	63	4	i aq
b336	2-Bromo-1-propene	$CH_3C(Br)=CH_2$	120.98	1,200	1.362_4^{20}	1.4425^{20}	-125	49	4	1
b337	2-Bromopropionic acid	CH ₃ CH(Br)COOH	152.98	2, 254	1.7000^{20}	1.4750^{20}	25.7	203	100	v s aq, alc, eth
b338	3-Bromopropionic acid	BrCH ₂ CH ₂ COOH	152.98	2, 256	1.480		62.5		65	s aq, alc, bz, chl, eth

b339	3-Bromopropionitrile	BrCH ₂ CH ₂ CN	133.98	$2^2, 231$	1.6152_4^{20}	1.4800^{20}		78 ^{10mm}	98	v s alc, eth
b340	2-Bromopropionyl	CH ₃ CH(Br)COCl	171.43	2, 256	1.70011	1.4800^{20}		133	51	d aq; s chl, eth
	chloride									
b341	3-Bromopropionyl	BrCH ₂ CH ₂ COCl	171.43	$2^2, 231$	1.701	1.4968^{20}		57 ^{17mm}	79	
	chloride									
b342	α-Bromopropio-	C ₆ H ₅ COCHBrCH ₃	213.08	7, 302	1.430_4^{20}	1.5715^{20}		250	>112	s alc, bz, eth, acet
	phenone									
b343	3-Bromopropyl	C ₆ H ₅ OCH ₂ CH ₂ CH ₂ Br	215.10	6, 142	1.365	1.5464^{20}	10-11	130-	96	
	phenyl ether							134 ^{14mm}		
b344	3-Bromopropyne	BrCH₂C≡CH	118.97	1, 248	1.335	1.4905^{20}		88–90	18	
b345	2-Brompyridine	BrC ₅ H ₄ N	158.00	20, 233	1.65718	1.5720^{20}		194	54	i aq; s org solv
b346	3-Bromopyridine	BrC ₅ H ₄ N	158.00	20, 233	1.645_4^0	1.5695^{20}	142-143	173	51	s aq; v s alc, eth
b347	3-Bromoquinoline		208.06	20, 363	1.533	1.6640^{20}	15	276	>112	s HOAc
b348	5-Bromosalicylic	Br(HO)C ₆ H ₃ COOH	217.02	10, 107			166			0.3 aq ⁸⁰ ; 85 alc ²⁵ ;
	acid									70 eth ²⁵
b349	β -Bromostyrene	C ₆ H ₅ CH=CHBr	183.05	5, 477	1.422_4^{20}	1.6066^{20}	7	112 ^{20mm}	79	i aq; misc alc, eth
b350	Bromosuccinic acid	HOOCCH ₂ CH(Br)COOH	196.99	2,621	2.073		172 d			18 aq; s alc

 β -Bromophenetole, b286

3-Bromopropene, a85

3-(Bromopropyl)benzene, b330

5-Bromopseudocumene, b361

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b351	N-Bromosuccinimide		177.99	21, 380	2.098		173 sl d			1.5 aq; 14.4 acet; 3.1 HOAc; 0.02 CCl ₄
b352	1-Bromotetradecane	H(CH ₂) ₁₄ Br	277.30	1 ² , 136	1.0124_4^{25}	1.4600^{20}	6	178 ^{20mm}	>112	s alc; v s chl; misc bz, acet
b353	2-Bromothiophene	$Br(C_4H_3S)$	163.04	17, 33	1.684_4^{20}	1.5860^{20}		151	60	v s acet, eth
b354	4-Bromothiophenol	BrC ₆ H ₄ SH	189.08	6, 330			76	239		
b355	2-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 304	1.422_{25}^{25}	1.552 ²⁵	-26	181	78	0.1 aq; misc alc, bz, chl, eth
b356	3-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 305	1.4099_4^{20}	1.5517^{20}	-39.8	183.7	60	s alc, bz, eth
b357	4-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 305	1.3959_{35}^{35}	1.5490	28.5	184.5	85	s alc, bz, eth
b358	Bromotri-	BrCCl ₃	198.28	1,67	1.997_{25}^{25}	1.5063	-21	103.8	none	misc org solv
	chloromethane									
b359	1-Bromotridecane	H(CH ₂) ₁₃ Br	263.27	1 ² , 134	1.0262_4^{20}	1.4592^{20}	7	150 ^{10mm}	>112	v s chl
b360	Bromotri- fluoromethane	BrCF ₃	148.92	13, 83	1.5800_4^{20}			-57.8		v s chl
b361	5-Bromo-1,2,4-tri- methylbenzene	$BrC_6H_2(CH_3)_3$	199.10	5, 403			73	235		i aq; s alc
b362	2-Bromo-1,3,5-tri- methylbenzene	$BrC_6H_2(CH_3)_3$	199.10	5, 408	1.301	1.5511 ²⁰	2	225	96	i aq; s bz; v s eth
b363	Bromotrimethyl- germane	(CH ₃) ₃ GeBr	197.60		1.54418	1.4705^{20}	-25	113.7		
b364	Bromotrimethylsilane	(CH ₃) ₃ SiBr	153.10		1.160	1.4145^{20}		79	1	
b365	Bromotriphenyl- ethylene	$(C_6H_5)_2C = C(Br)C_6H_5$	335.22				114–115			
b366	Bromotriphenyl- methane	$(C_6H_5)_3CBr$	323.24	5, 704			152–154	230 ^{15mm}		
b367	11-Bromoundecanoic acid	Br(CH ₂) ₁₀ COOH	265.20	2 ² , 315			51	174 ^{2mm}		i aq; v s alc

b368	α -Bromo- o -xylene	BrCH ₂ C ₆ H ₄ CH ₃	185.07	5, 365	1.381^{23}	1.5742^{20}	21	223-224	82	s alc, eth
b369	α -Bromo- m -xylene	BrCH ₂ C ₆ H ₄ CH ₃	185.07	5, 374	1.370^{23}	1.5560^{20}		185 ^{340mm}	82	s alc, eth
b370	2-Bromo-p-xylene	$BrC_6H_3(CH_3)_2$	185.07	5, 385	1.340	1.5505^{20}	9-10	199-201	79	
b371	4-Bromo-o-xylene	$BrC_6H_3(CH_3)_2$	185.07	5, 365	1.370_{15}^{15}	1.5560^{20}		215	80	v s alc, eth
b372	Brucine		394.45	$27^2,797$			178			77 alc; 1 bz; 20 chl
b373	1,2-Butadiene	CH ₃ CH=C=CH ₂	54.09	1, 249	0.676_4^{10}	1.42051	-136.2	10.9		misc alc, eth
b374	1,3-Butadiene	CH ₂ =CHCH=CH ₂	54.09	1, 249	0.650_4^{-6}	1.4293^{-25}	-108.9	-4.4		misc alc, eth
b375	1,3-Butadienyl	CH ₃ C(=O)OCH=CH-	112.13	$2^3, 295$	0.945	1.4690^{20}		$60^{40 \text{mm}}$	33	
	acetate	CH=CH ₂								
b376	1,3-Butadiyne	HC≡CC≡CH	50.06	1^3 , 1056	0.7364_4^0	1.4189 ⁵	-36	10.3		v s eth; s bz, acet
b377	2-Butanamine	CH ₃ CH ₂ CH(NH ₂)CH ₃	73.14	4, 160	0.7308_4^{15}	1.396315	-104.5	66	-19	misc aq, alc
b378	Butane	CH ₃ CH ₂ CH ₂ CH ₃	58.12		0.6011^{0}	1.3562^{-13}	-138.3	-0.50		
b379	1,4-Butanediamine	H ₂ NCH ₂ CH ₂ CH ₂ CH ₂ NH ₂	88.15	4, 264	0.877_4^{25}	1.4569^{20}	27-28	158-160	51	s aq
b380	Butanedinitrile	NCCH ₂ CH ₂ CN	80.09	2,615	0.9867_4^{60}	1.4173^{60}	57.9	265-267		11.5 aq; s acet,
										chl, diox; sl s
										bz, eth
b381	1,2-Butanediol	CH ₃ CH ₂ CH(OH)CH ₂ OH	90.12	1,477	1.006_0^{18}	1.4380^{20}		207.5	93	s aq, alc, acet
b382	1,3-Butanediol	CH ₃ CH(OH)CH ₂ CH ₂ OH	90.12	1,477	1.0053_{20}^{20}	1.441^{20}	<-50	207.5	121	s aq, alc, acet; 9
										eth

 α -Bromotoluene, b85

Bromo- α , α , α -trifluorotoluenes, b233, b234

3-Bromo-1,7,7-trimethylbicyclo[2.2.1]heptane-2-one, b245

4-Bromoveratrole, b268

4-Bromo-2,6-xylenol, b270

BSA, b207

BSTFA, b212

BTMSA, b208

Busulfan, b188

Butanedioic acid, s14

 α -Butadiene sulfone, d368

1,4-Butanediol diglycidyl ether, b175

1,4-Butanediol dimethanesulfonate, b188

$$O \xrightarrow{Br} O$$

$$O \xrightarrow{b351}$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b383	1,4-Butanediol	HOCH ₂ CH ₂ CH ₂ CH ₂ OH	90.12	1, 478	1.016 ²⁵	1.4452 ²⁰	120.9	230	>112	misc aq, alc, acet; 0.3 bz; 3.1 eth; 0.9 PE
b384	meso-2,3-Butanediol	CH ₃ CH(OH)CH(OH)CH ₃	90.12	1, 479	0.9939_4^{25}	1.4324^{35}	34.4	182	85	misc aq, alc
b385	D-(-)-2,3-Butanediol	CH ₃ CH(OH)CH(OH)CH ₃	90.12	$1^2,546$	0.9869_4^{25}	1.4315^{25}	19.7	180 ^{715mm}	85	misc aq, alc; s eth
b386	2,3-Butanedione	CH ₃ C(O)C(O)CH ₃	86.09	1,769	0.990_{15}^{15}	1.3951^{20}		88	26	25 aq; misc alc,
										eth
b387	1,4-Butanedithiol	HSCH ₂ CH ₂ CH ₂ CH ₂ SH	122.25	1, 479	1.042	1.5290^{20}		106 ^{30mm}	70	i aq; v s alc
b388	1-Butanethiol	CH ₃ CH ₂ CH ₂ CH ₂ SH	90.19	1,370	0.8367_4^{25}	1.4403^{25}	-115.7	98.5	12	0.06 aq; v s alc, eth
b389	2-Butanethiol	CH ₃ CH ₂ CH(SH)CH ₃	90.19	1, 373	0.8246_4^{25}	1.4338^{25}	-165	85.0	21	sl s aq; v s alc, eth
b390	1,2,4-Butanetriol	HOCH ₂ CH ₂ CH(OH)- CH ₂ OH	106.12	1,519	1.018 ²⁰	1.4748 ²⁰		191 ^{18mm}	167	v s aq, alc
b391	1-Butanol	CH ₃ CH ₂ CH ₂ CH ₂ OH	74.12	1, 367	0.8097_4^{20}	1.3993^{20}	-88.6	117.7	35	7.4 aq; misc alc, eth
b392	2-Butanol	CH ₃ CH ₂ CH(OH)CH ₃	74.12	1, 371	0.8069_4^{20}	1.3972 ²⁰	-114.7	99.5	26	12.5 aq; misc alc, eth
b393	2-Butanone	CH ₃ CH ₂ COCH ₃	72.11	1 ² , 726	0.8049_4^{20}	1.3788 ²⁰	-86.7	79.6	-3	24 aq; misc alc, bz, eth
b394	2-Butanone oxime	CH ₃ CH ₂ C (=NOH)CH ₃	87.12	$1^2,730$	0.9232_4^{20}	1.4428	-29.5	72 ^{25mm}		s aq; misc alc, eth
b395	1-Butene	CH ₃ CH ₂ CH=CH ₂	56.10	$1^3,715$	0.62554-185	1.3962^{20}	-185.3	-6.3		i aq; v s alc, eth
b396	cis-2-Butene	CH ₃ CH=CHCH ₃	56.10	$1^3,728$	0.6213_4^{20}	1.3931^{-25}	-138.9	3.7		i aq; v s alc, eth
b397	trans-2-Butene	CH ₃ CH=CHCH ₃	56.10	$1^3,730$	0.6041_4^{20}	1.3848^{-25}	-105.6	0.88		i aq; v s alc, eth
b398	cis-2-Butene-1,4-diol	HOCH ₂ CH=CHCH ₂ OH	88.11	$1^2, 567$	0.0700_4^{20}	1.4793^{20}	12.5	234	128	s aq; v s alc
b399	trans-2-Butene-1,4-diol	HOCH ₂ CH=CHCH ₂ OH	88.11	1 ³ , 2252	0.070_4^{20}	1.4779^{20}	27.3	132		v s aq, alc
b400	3-Butenenitrile	H ₂ C=CHCH ₂ CN	67.09	2, 408	0.8341_4^{20}	1.4060^{20}	-87	119	21	sl s aq; misc alc, eth
b401	cis-2-Butenoic acid	CH₃CH=CHCOOH	86.09	2,412	1.0267_4^{20}	1.448214	14	168–169		v s aq; s alc

b402	trans-2-Butenoic acid	CH ₃ CH=CHCOOH	86.09	2,408	0.964_4^{80}	1.4228 ⁷⁷	71.4	185.0	87	54.6 aq; v s EtOH, bz, acet
b403	3-Butenoic acid	H ₂ C=CHCH ₂ COOH	86.09	2,407	1.0091_4^{20}	1.4249^{20}	-39	163	65	s aq; misc alc, eth
b404	cis-2-Buten-1-ol	CH ₃ CH=CHCH ₂ OH	72.11	1,442	0.8662_4^{20}	1.4342^{20}	-89.4	123.6	56	16.6 aq; misc alc
b405	trans-2-Buten-1-ol	CH ₃ CH=CHCH ₂ OH	72.11	1,442	0.8454_4^{20}	1.4289^{20}		121.2	56	16.6 aq; misc alc
b406	3-Buten-2-one	H ₂ C=CHCOCH ₃	70.09	1,728	0.8636_4^{20}	1.4086^{20}		81.4	-6	v s aq, alc, acet,
										eth
b407	1-Buten-3-yne	HC≡CCH=CH ₂	52.07	1 ³ , 1032	0.7095_4^1	1.4161^{1}		5.1		
b408	4-Butoxyaniline	CH ₃ (CH ₂) ₃ OC ₆ H ₄ NH ₂	165.24	13 ² , 226	0.992	1.5343^{20}		148-		
								149 ^{13mm}		
b409	4-Butoxybenzoic acid	CH ₃ (CH ₂) ₃ OC ₆ H ₄ COOH	194.23	$10^2, 93$			150			
b410	2-Butoxyethanol	CH ₃ (CH ₂) ₃ OCH ₂ CH ₂ OH	118.18	$1^2,519$	0.9012_4^{20}	1.4198^{20}	-40	170.2	60	5 aq; s most org
										solv
b411	2-(2-Butoxyethoxy)-	HOCH ₂ CH ₂ OCH ₂ -	162.23	$1^2,521$	0.9536_{20}^{20}	1.4306^{20}	-68.1	230.4	110	misc aq, alc, bz,
	ethanol	CH ₂ OC ₄ H ₉								acet, PE, CCl ₄
b412	Butyl acetate	C ₄ H ₉ OOCCH ₃	116.16	2, 130	0.8813_4^{20}	1.3941^{20}	-73.5	126.1	37	0.43 aq; misc alc,
										eth; s most org
					25					solv
b413	DL-sec-Butyl acetate	CH ₃ COOCH(CH ₃)C ₂ H ₅	116.16	2^2 , 141	0.865_4^{25}	1.3840^{25}		112.3	32	0.62 aq; s alc, eth
b414	tert-Butyl acetate	(CH ₃) ₃ COOCCH ₃	116.16	2, 131	0.8665_4^{20}	1.3853^{20}		97.8	15	i aq; misc alc, eth
b415	tert-Butyl aceto-	$(CH_3)_3COC(=O)CH_2$ -	158.20		0.954	1.4180^{20}			60	
	acetate	$C(=O)CH_3$		-2						l
b416	Butyl acrylate	$H_2C = CHCOOC_4H_9$	128.17	2^2 , 388	0.894_{16}^{25}	1.4160		148	38	i aq; s alc, eth
b417	Butylamine	CH ₃ CH ₂ CH ₂ CH ₂ NH ₂	73.14	4, 156	0.7327_4^{25}	1.3992^{25}	-50.5	77.9	-1	misc aq, alc, eth,
					0 50 7 1 20					PE
b418	tert-Butylamine	$(CH_3)_3CNH_2$	73.14	4, 173	0.6951_4^{20}	1.3788^{20}	-67.5	44.4	-8	misc aq, alc
b419	2-(tert-Butylamino)-	(CH ₃) ₃ CNHCH ₂ CH ₂ OH	117.19				42–45	90-92 ^{25mm}	68	
	ethanol									

(*E*)-2-Butenal, c282 Buten-4-carboxylic acid, p50 Butopyronoxyl, b445 Butoxybenzene, b477 1-Butoxybutane, d115 Butyl alcohols, b393, b392, m382 sec-Butylamine, b377

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b420	3-(tert-Butylamino)-	(CH ₃) ₃ CNHCH ₂ CH(OH)-	147.22				70	92 ^{1mm}		
	1,2-propanediol	CH ₂ OH								
b421	4-Butylaniline	CH ₃ CH ₂ CH ₂ CH ₂ - C ₆ H ₄ NH ₂	149.24	12 ¹ , 503	0.945	1.5350^{20}		120 ^{15mm}	101	
b422	2- <i>tert</i> -Butylanthra- quinone		264.32				100			
b423	Butylbenzene	CH ₃ CH ₂ CH ₂ CH ₂ C ₆ H ₅	134.22	5, 413	0.8604_4^{20}	1.4898^{20}	-88	183.3	59	misc alc, bz, eth
b424	sec-Butylbenzene	CH ₃ CH ₂ CH(CH ₃)C ₆ H ₅	134.22	5, 414	0.8608_4^{20}	1.4902^{20}	-82.7	173.3	45	misc alc, bz, eth
b425	tert-Butylbenzene	(CH ₃) ₃ CC ₆ H ₅	134.22	5, 415	0.8669_4^{20}	1.4927^{20}	-57.9	169.1	34	misc alc, bz, eth
b426	Butyl benzoate	C ₆ H ₅ COOC ₄ H ₉	178.23	9, 112	1.000^{20}	1.496	-22	250		i aq; s alc, eth
b427	4- <i>tert</i> -Butylbenzoic acid	(CH ₃) ₃ CC ₆ H ₄ COOH	178.23	9, 560			167			i aq; v s alc, bz
b428	4- <i>tert</i> -Butylbenzoyl chloride	(CH ₃) ₃ CC ₆ H ₄ COCl	196.68		1.007	1.5364 ²⁰		135 ^{20mm}	87	
b429	N-(tert-Butyl)benzyl-	C ₆ H ₅ CH ₂ NHC(CH ₃) ₃	163.27	12, 1022	0.881	1.4968 ²⁰		80 ^{5mm}	80	
b430	Butyl butyrate	CH ₃ CH ₂ CH ₂ COOC ₄ H ₉	144.21	2, 271	0.8717_{20}^{20}	1.4035		156.9	51	i aq; misc alc, eth
b431	tert-Butyl carbazate	H ₂ NNHCOOC(CH ₃) ₃	132.16		20		42	65 ^{0.03mm}		
b432	4-tert-Butylcatechol	(CH ₃) ₃ CC ₆ H ₃ (OH) ₂	166.22		1.049 ⁶⁰ ₂₅		55	285	151	0.2 aq ⁸⁰ ; 240 eth ²⁵ ; s alc; v s
										acet
b433	tert-Butyl chloro- acetate	CICH ₂ COOC(CH ₃) ₃	150.61	$2^3,444$	1.053	1.4230^{20}		48–49 ^{11mm}	41	
b434	4- <i>tert</i> -Butyl-1-chlorobenzene	(CH ₃) ₃ CC ₆ H ₄ Cl	168.67	5, 416	1.006	1.5108 ²⁰	23–25	217		
b435	tert-Butylchlorodi- phenylsilane	$(CH_3)_3CSi(C_6H_5)_2Cl$	274.87		1.057	1.5675 ²⁰		90 ^{0.02mm}	>112	
b436	Butyl chloroformate	ClCOOC ₄ H ₉	136.58	$3^2, 11$	1.074_4^{25}	1.4114 ²⁰		142	25	d aq, alc; misc eth

b437	S-tert-Butyl chloro- thioformate	$CIC(=O)SC(CH_3)_3$	152.6		1.081 ₄ ³⁰	1.469130		42.0 ^{10mm}	46	
b438	tert-Butyl cyano- acetate	NCCOOC(CH ₃) ₃	141.17			1.4200^{20}		108		
b439	2- <i>tert</i> -Butylcyclo-hexanol	$(CH_3)_3CC_6H_{10}OH$	156.27		0.902		46			i aq
b440	4- <i>tert</i> -Butylcyclo-hexanol	$(CH_3)_3CC_6H_{10}OH$	156.27	6 ¹ , 18			70	115 ^{15mm}	105	i aq
b441	2- <i>tert</i> -Butylcyclo-hexanone	(CH3)3CC6H9(=O)	154.25	7 ³ , 143	0.896	1.4565^{20}		62.5 ^{4mm}		
b442	4- <i>tert</i> -Butylcyclo-hexanone	(CH3)3CC6H9(=O)	154.25	7 ¹ , 29			50	116 ^{20mm}	96	i aq
b443	Butyl decyl- o-phthalate	C ₄ H ₉ OOCC ₆ H ₄ COO- C ₁₀ H ₂₁	362.51		0.994_{25}^{25}				202	
b444	N-Butyldiethanol-	$C_4H_9N(CH_2CH_2OH)_2$	161.25	4, 285	0.986_{20}^{20}	1.4625 ²⁰	<-70	276	126	
b445	Butyl 3,4-dihydro-2,2-dimethyl-4-oxo-2 <i>H</i> -		226.27		1.05425	1.4767 ²⁰		256–270	>112	misc alc, chl, eth
	pyran-6-carboxylate									

Butyl bromides, b238, b239, b311 N-Butyl-1-butanamine, d107 Butyl carbitol, b411 Butyl Cellosolve, b410 Butyl chlorides, c64, c65, c162 2-tert-Butyl-o-cresol, b462

2-*tert*-Butyl-*p*-cresol, b461 *tert*-Butyldihydroxybenzene, b432

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b446	tert-Butyldimethyl-	(CH ₃) ₃ CSi(CH ₃) ₂ Cl	150.7				91.5	124–126		
	chlorosilane									
b447	1,3-Butylene	CH ₃ CH(OOCCH ₃)CH ₂ -	174.20	2, 143	1.028	1.4199^{20}		99 ^{8mm}	85	v s aq; s alc
1 440	diacetate	CH ₂ OOCCH ₃	11710		0.0020	4 4 4 4 2 0	2.5	400		
b448	<i>N</i> -Butylethanolamine	HOCH ₂ CH ₂ NHC ₄ H ₉	117.19		0.89^{20}	1.444 ²⁰	-3.5	192	77	
b449	Butyl ethyl ether	$C_4H_9OC_2H_5$	102.18	1^3 , 1502	0.7495_4^{20}	1.381820	-103	92.5		i aq; misc alc, eth
b450	2-Butyl-2-ethyl-1,3- propanediol	$HOCH_2C(C_2H_5)(C_4H_9)-$ CH_2OH	160.25		0.931_{20}^{50}	1.4587 ²⁵	41.4	195 ^{100mm}		0.8 aq
b451	Butyl ethyl sulfide	$C_4H_9SC_2H_5$	118.24	1^3 , 1522	0.8376_4^{20}	1.4491^{20}	-95.1	144.2		s chl
b452	tert-Butylhydrazine HCl	(CH ₃) ₃ CNHNH ₂ HCl	124.61	4 ³ , 1734			191–174			
b453	tert-Butylhydroper-	(CH ₃) ₃ C—O—OH	90.12		0.896_4^{20}	1.4007^{20}	4–5	33-4 ^{17mm}	62	s aq, alc, chl, eth
	oxide									•
b454	tert-Butylhydro- quinone	$(CH_3)_3CC_6H_3(OH)_2$	166.22				129			
b455	Butyl isocyanate	CH ₃ CH ₂ CH ₂ CH ₂ NCO	99.13		0.880	1.4061^{20}		115	26	
b456	tert-Butyl isocyanate	(CH ₃) ₃ CNCO	99.13	4, 175	0.868	1.3865^{20}		86	26	
b457	Butyllithium	CH ₃ CH ₂ CH ₂ CH ₂ Li	64.06					80 ^{0.0001mm}	pyro-	
									pho-	
									ric	
b458	tert-Butyllithium	(CH ₃) ₃ CLi	64.06					subl	pyro-	
								70 ^{0.1mm}	pho-	
					2.5				ric	
b459	Butyl methacrylate	$H_2C = C(CH_3)COOC_4H_9$	142.19		0.889_{15}^{25}	1.4220^{25}		170	49	i aq; misc alc, eth
b460	tert-Butyl methyl ether	(CH ₃) ₃ COCH ₃	88.15	1, 381	0.758	1.3685 ²⁰	-109	56	-10	s aq; v s alc, eth
b461	2- <i>tert</i> -Butyl-4- methylphenol	(CH ₃) ₃ CC ₆ H ₃ (CH ₃)OH	164.25		0.9247 ₄ ⁷⁵	1.4969 ⁷⁵	51.7	237		i aq; s org solv

b462	2-tert-Butyl-6-	(CH ₃) ₃ CC ₆ H ₃ (CH ₃)OH	164.25	I	I	1.519520	32	230	107	I
0402	methylphenol	(CH ₃) ₃ CC ₆ H ₃ (CH ₃)OH	104.23			1.3193	32	230	107	
b463	Butyl methyl sulfide	$C_4H_9SCH_3$	104.21	1 ³ , 1521	0.8426_4^{20}	1.4477^{20}	-97.8	123.4		v s alc
b464	Butyl nitrite	C ₄ H ₉ ONO	103.12	1, 369	0.9114_4^0	1.3768		78	4	misc alc, eth
b465	tert-Butyl nitrite	(CH ₃) ₃ CONO	103.12	1 ² , 415	0.8671_4^{20}	1.3687 ²⁰		63		sl s aq; v s alc, chl, eth, CS ₂
b466	Butyl octadecanoate	CH ₃ (CH ₂) ₁₆ COOC ₄ H ₉	340.60	$2^2,352$	0.8551_4^{20}	1.4422^{25}	26.3	343	160	s alc, v s acet
b467	Butyl 4-oxopent- anoate	$CH_3C(=O)CH_2-$ $CH_2COOC_4H_9$	172.22		0.9735_4^{20}	1.4270 ²⁰		107 ^{6mm}	91	s alc, eth, acet
b468	tert-Butyl peroxy- benzoate	$C_6H_5(=O)O-OC(CH_3)_3$	194.23		1.021	1.4990 ²⁰		76 ^{0.2mm}	93	
b469	2-sec-Butylphenol	CH ₃ CH ₂ CH(CH ₃)- C ₆ H ₄ OH	150.22		0.982	1.522220	12	228	112	i aq; s alc; v s eth
b470	2-tert-Butylphenol	(CH ₃) ₃ CC ₆ H ₄ OH	150.22	$6^2,489$	0.9783_4^{20}	1.5228^{20}	-7	221-224	110	
b471	3-tert-Butylphenol	(CH ₃) ₃ CC ₆ H ₄ OH	150.22				40-41	240		
b472	4-sec-Butylphenol	CH ₃ CH ₂ CH(CH ₃)- C ₆ H ₄ OH	150.22	6, 522	0.969_4^{20}	1.5150	62	136 ^{25mm}	115	s hot aq, alc, eth
b473	4-tert-Butylphenol	(CH ₃) ₃ CC ₆ H ₄ OH	150.22	6, 524	0.908_4^{114}	1.4787114	100-101	237		i aq; s alc, eth
b474	2-(4- <i>sec</i> -Butylphen-oxy)ethanol	CH ₃ CH ₂ CH(CH ₃)C ₆ H ₄ - OCH ₂ CH ₂ OH	194.2		1.008 ²⁵		<-20	158 ^{10mm}	149	0.1 aq
b475	2-(4- <i>tert</i> -Butylphen- oxy)ethanol	(CH ₃) ₃ CC ₆ H ₄ - OCH ₂ CH ₂ OH	194.3		1.016 ²⁵		54	167 ^{10mm}	157	0.1 aq
b476	tert-Butyl phenyl carbonate	$C_6H_5OC(=O)OC(CH_3)_3$	194.23		1.047	1.4805 ²⁰		79 ^{0.8mm}		
b477	Butyl phenyl ether	CH ₃ CH ₂ CH ₂ CH ₂ OC ₆ H ₅	150.22	6, 143	0.9351_4^{20}	1.4970^{20}	-19	210.3	82	

Butyl disulfides, d113, d114

1,4-Butylene bis(2,3-epoxypropyl) ether, b175

1,3-Butylene glycol methyl ether, m57

1,2-Butylene oxide, e3 Butyl ether, d115 Butyl ethyl ketone, h16 tert-Butyl fluoride, f20 Butyl glycol, b410 2,2'-(Butylimino)diethanol, b444 Butyl iodides, i30, i31, i44

Butyl levulinate, b467 Butyl mercaptans, b388, m378, m379, m380 Butyl methyl ketone, d497 *tert*-Butyl perbenzoate, b468

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b478	4-tert-Butylphenyl salicylate	HOC ₆ H ₄ COOC ₆ H ₄ - C(CH ₃) ₃	270.31				62–64			0.1 aq; 79 alc; 153 EtAc; 158 toluene
b479	Butyl propionate	CH ₃ CH ₂ COOC ₄ H ₉	130.19	2, 241	0.8818^{15}	1.3982^{25}	-89.6	145.5		misc alc, eth
b480	4- <i>tert</i> -Butylpyridine	$(CH_3)_3C(C_5H_4N)$	135.21	20, 252	0.915	1.4952^{20}		197	63	
b481	Butyltin chloride	C ₄ H ₉ SnCl ₃	282.17		1.693	1.5229^{20}		93 ^{10mm}	81	
b482	4- <i>tert</i> -Butyltoluene	(CH ₃) ₃ CC ₆ H ₄ CH ₃	148.25	5, 439	0.853	1.4897^{20}		192	54	
b483	Butyltrichlorosilane	C ₄ H ₉ SiCl ₃	191.5	4 ¹ , 582	1.161_4^{20}	1.436^{20}		142-143		d aq, hot alc; s eth
b484	Butyl trifluoro- acetate	CF ₃ COOC ₄ H ₉	170.1		1.0268 ²²	1.353^{22}		100.2		
b485	Butyltrimethoxysilane	$C_4H_9Si(OCH_3)_3$	178.3		0.9312_4^{20}	1.3979^{20}		164–165		
b486	tert-Butyl tri- methylsilyl peroxide	(CH ₃) ₃ C—O—O—Si- (CH ₃) ₃	162.3		0.8219420	1.3935 ²⁵	d 135	41 ^{41mm}		
b487	Butyl urea	C ₄ H ₀ NHCONH ₂	116.16	41,371			93–95			s aq, alc, eth
b488	Butyl vinyl ether	C ₄ H ₀ OCH=CH ₂	100.16	.,	0.7792^{20}	1.4007^{20}	-112.7	94.2	_9	0.3 aq
b489	5-tert-Butyl-m- xylene	$(CH_3)_3CC_6H_3(CH_3)_2$	162.28	5, 447	0.867	1.4946^{20}		205–206	72	
b490	1-Butyne	CH₃CH₂C≡CH	54.09	1, 249	0.7110_4^{-31}	1.3962^{20}	-125.7	8.1		i ag; s alc, eth
b491	2-Butyne	CH₃C≡CCH₃	54.09	1, 249	0.6910_4^{20}	1.3920^{20}	-32.3	17.0		i ag; s alc, eth
b492	2-Butyne-1,4-diol	HOCH ₂ C≡CCH ₂ OH	86.09	11, 261		1.450 ²⁵	54–58	238	152	374 aq; 83 alc; 0.04 bz; 2.6 eth; 70 acet
b493	Butyraldehyde	CH ₃ CH ₂ CH ₂ CHO	72.11	1,662	0.8016_4^{20}	1.3791 ²⁰	-96.4	74.8	-6.7	7.1 aq; misc alc, eth, acet, EtAc
b494	Butyramide	CH ₃ CH ₂ CONH ₃	87.12	2, 275			116	216		16 aq; s alc
b495	Butyric acid	CH ₃ CH ₂ CH ₂ COOH	88.11	2, 264	0.9582_4^{20}	1.3980^{20}	-5.3	163.3	77	misc aq, alc, eth
b496	Butyric anhydride	[CH ₃ CH ₂ CH ₂ C(O)] ₂ O	158.20	2, 274	0.9668_4^{70}	1.4130^{20}	-65.7	199.5	87	s aq, alc(d), eth
		I	I	I		l	l		I	

b497	3-Butyrolactone		86.09	17 ¹ , 130	1.056	1.4109	20	73 ^{29mm}	60	l
b498	4-Butyrolactone		86.09	17, 234	1.124_4^{25}	1.4348 ²⁵	-43.5	204	98	misc aq, alc, acet, bz, eth, CCl ₄
b499	Butyronitrile	CH ₃ CH ₂ CH ₂ CN	69.11	$2^2, 252$	0.7954_4^{15}	1.386015	-111.9	117.9	16	3.3 aq; misc alc, eth
b500	Butyrophenone	$C_6H_5C(O)C_3H_7$	148.21	7, 313	1.021	1.5195^{20}	13	222	88	
b501	Butyryl chloride	CH ₃ CH ₂ CH ₂ COCl	106.55	2, 274	1.0263421	1.4122 ²⁰	-89	102	21	s aq, alc(d); misc eth
c1	Caffeine		194.19	26, 461	1.2348		238	subl 178		2.1 aq; 1.5 alc; 18 chl; 0.19 eth; 1 bz
c2	DL-Camphene		136.24	5, 156	0.8422_4^{54}	1.455154	51-52	159	36	i aq; s alc, chl, eth
c3	D-(+)-Camphor		152.23	7, 101	0.9920_4^{25}		178.8	207.4		100 alc; 100 eth; 200 chl; 250 acet
c4	DL-Camphor		152.24	7, 135			177	204	64	
c5	D-Camphoric acid		200.23	9,745	1.186_4^{20}		186–188			4 aq; 100 alc; s chl, eth

Butyl o-phthalate, d128 Butyl propyl ketone, 036 Butyl stearate, b466 Butyl sulfate, d131 Butyl sulfides, d132, d133 Butyl sulfite, d134 Butyl sulfone, d135 Butyrolactam, p275

Cadaverine, p29 2-Camphanone, c3

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c6	DL-Camphoric		182.22	17, 455	1.19420		225	270		s bz; sl s aq, alc,
c7	anhydride D-10-Camphor- sulfonic acid		250.32	11, 316			194 d			eth deliq moist air; sl s HOAc, EtAc;
	hydrate									i eth
c8	Carbazole		167.21	20, 433			245–246	355		
c9	4-Carbethoxy-3- methyl-3-cyclo- hexen-1-one		182.22	10, 631	1.078	1.4880 ²⁰		268–272	>112	
c10	Carbobenzyloxy- glycine	C ₆ H ₅ CH ₂ OC(=O)NH- CH ₂ COOH	209.20				122			
c11	Carbohydrazide	$H_2NNHC(=O)NHNH_2$	90.09	3, 121			d 153			v s aq; i alc, bz, eth
c12	2-(Carbomethoxy)- ethylmethyl- dichlorosilane	CH ₃ OC(=0)CH ₂ CH ₂ Si- (CH ₃)Cl ₂	201.1		1.187 ₄ ²⁵	1.4439 ²⁵		98–99 ^{25mm}		
c13	2-Carbomethoxyethyl- trichlorosilane	CH ₃ OC(=O)CH ₂ CH ₂ - SiCl ₃	221.6		1.325420	1.448 ²⁰		88-89 ^{2mm}		
c14	2-Carboxybenz- aldehyde	HC(=O)C ₆ H ₄ COOH	150.13	10,666			96–98			
c15	4-Carboxy-1,2-benzenedicarboxylic anhydride		192.13	18, 468			161–164	240– 245 ^{14mm}		15.5 DMF; 49.6 acet; 21.6 EtAc
c16	4-Carboxybenzene- sulfonamide	HOOCC ₆ H ₄ SO ₂ NH ₂	201.20	11, 390			d 280			i aq, bz, eth; v s alc
c17	2-Carboxyethyl- phosphonic acid	HOOCCH ₂ CH ₂ - P(O)(OH) ₂	154.06	$4^2,976$						
c18	DL-Carnitine HCl	(CH ₃) ₃ NCH ₂ CHOH- CH ₂ COOH·HCl	197.66				197 d			v s aq; i acet, eth

c19	trans-β-Carotene	536.89	30, 87	1.000_{20}^{20}		183			i aq; s bz, chl, CS ₂
c20	D-(+)-Carvone	150.22	7, 153	0.965_4^{20}	1.4989^{20}		230	88	i aq; misc alc
c21	Catecholborane	119.92			1.5070^{20}	12	50 ^{50mm}		

Caprylaldehyde, o40

Caprylonitrile, o27
Capryloyl chloride, o37
CAPS, c337
N-(Carbamoylmethyl)iminodiacetic acid, a14
Carbamylurea, b215
Carbanilide, d693
Carbazole, d665
Carbitol, e35
Carbitol acetate, e36
Carbobenzoxy chloride, b90
4,4'-Carboxyldiphthalic anhydride, b55

[Note: 9 successive () units]

N-Carbonylsulfamyl chloride, c240
Carboxybenzaldehyde, f33
(3-Carboxy-2-hydroxypropyl)
trimethylammonium hydroxide, c18
3-Carbomethoxypropionyl chloride, m188
(Carboxymethylimino)bis(ethylenenitrilo)tetraacetic acid, d299
(Carboxylmethyl)trimethylammonium
hydroxide, b128
3-Carboxypropyl disulfide, d708

1.15

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c22	2-Chloroacetamide	CICH ₂ CONH ₂	93.51	2, 199			118	225 d		10 aq; 10 alc; sl s
c23	<i>p</i> -Chloroacetanilide	CIC ₆ H ₄ NHCOCH ₃	169.61	12, 611	1.385 ²⁰		179			i aq; v s alc, eth, CS ₂
c24	Chloroacetic acid	CICH₂COOH	94.50	2, 194	1.580(c)	1.429765	63(α)	189		v s aq; s alc, bz, eth
c25	Chloroacetic anhydride	[ClCH ₂ C(O)] ₂ O	170.98	2, 199	1.5494420		46	203		d aq; v s chl, eth
c26	<i>p</i> -Chloroacetoacet-anilide	CH ₃ COCH ₂ CONHC ₆ H ₄ Cl	211.65				134			
c27	Chloroacetonitrile	CICH,CN	75.50	2, 201	1.193	1.4225^{20}		126	47	
c28	α-Chloroaceto- phenone	C ₆ H ₅ COCH ₂ Cl	154.60	7, 282	1.32415		54	245		i aq; v s alc, bz, eth
c29	o-Chloroaceto- phenone	ClC ₆ H ₄ COCH ₃	154.60	7 ¹ , 151	1.188	1.5438 ²⁰		228 ^{738mm}	88	sl s aq; s eth
c30	p-Chloroaceto- phenone	ClC ₆ H ₄ COCH ₃	154.60	7, 281	1.192_4^{20}	1.5549	20–21	237	90	i aq; misc alc, eth
c31	Chloroacetyl chloride	ClCH₂COCl	112.94	2, 199	1.41825	1.4530 ²⁰	-22.5	106	none	d aq, MeOH
c32	2-Chloroacrylo- nitrile	$H_2C = C(Cl)CN$	87.51		1.096	1.4290 ²⁰	-65	89	6	
c33	2-Chloroaniline	ClC ₆ H ₄ NH ₂	127.57	12, 597	1.2125_4^{20}	1.5881 ²⁰	-1.94	208.8	97	0.88 aq; s alc, bz, eth
c34	3-Choroaniline	ClC ₆ H ₄ NH ₂	127.57	12,602	1.2150_4^{22}	1.593120	-10.4	230.5	123	i aq; s alc, bz, eth
c35	<i>p</i> -Chloroaniline	CIC ₆ H ₄ NH ₂	127.57	12,607	1.169477	1.554685	72.5	232		s hot aq; v s alc, acet, eth, CS ₂
c36	1-Chloroanthra- quinone		242.66	7,787			160	subl		sl s alc; misc eth; s hot bz
c37	2-Chloroanthra-		242.66	7, 787			211	subl		sl s alc, bz; i eth
	quinone									

c38	2-Chlorobenz- aldehyde	CIC ₆ H ₄ CHO	140.57	7, 233	1.2483420	1.5658	11	215	87	sl s aq; s alc, bz, eth
20	_	CIC II CIIO	1.40.57	7.225	1 10/61	1 55061	47	21.4	0.7	
c39	4-Chlorobenz-	ClC ₆ H ₄ CHO	140.57	7, 235	1.196_4^{61}	1.552^{61}	47	214	87	s aq; v s alc, bz,
	aldehyde									eth
c40	2-Chlorobenzamide	CIC ₆ H ₄ CONH ₂	155.58	9, 336			142-144			
c41	Chlorobenzene	C ₆ H ₅ Cl	112.56	5, 199	1.1063^{20}	1.5248^{20}	-45.3	131.7	23	0.049 aq ³⁰ ; v s alc,
										bz, chl, eth
c42	4-Chlorobenzene-	ClC ₆ H ₄ SO ₂ NH ₂	191.64	11,55			146			s hot aq, hot alc,
	sulfonamide									hot eth
c43	4-Chlorobenzene-	ClC ₆ H ₄ SO ₂ Cl	211.07	11,55			55	141 ^{15mm}		d aq, alc; v s bz,
	sulfonyl chloride			,						eth
c44	4-Chlorobenzhydrol	CIC ₆ H ₄ CH(OH)C ₆ H ₅	218.68	6,680			58-60			
c45	2-Chlorobenzoic	ClC ₆ H ₄ COOH	156.57	9, 334	1.544_4^{25}		142			0.11 aq; v s alc, eth
	acid				1					

Cellosolve, e34 Cellosolve acetate, e37 Cetyl alcohol, h36 Cetyl bromide, b294 Chalcone, d686 CHES, c335 Chloramine T, c247 Chloranils, t24, t25 Chloranilic acid, d172 Chlorendic anhydride, h30 Chloroacetaldehyde diethyl acetal, c81 Chloroacetaldehyde dimethyl acetal, c89 Chloroacetone, c215 4-(Chloroacetyl)catechol, c86 Chloroanthranilic acid, a140 5-Chloroanthranilonitrile, a141 p-Chlorobenzenethiol, c243

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c46	3-Chlorobenzoic	CIC ₆ H ₄ COOH	156.57	9, 337	1.49625		157–158			0.04 aq; v s alc, eth
c46a c47 c48 c49	4-Chlorobenzoic acid 2-Chlorobenzonitrile 4-Chlorobenzonitrile 2-Chlorobenzo- phenone	CIC ₆ H ₄ COOH CIC ₆ H ₄ CN CIC ₆ H ₄ CN CIC ₆ H ₄ COC ₆ H ₅	156.57 137.57 137.57 216.67	9, 340 9, 336 9, 341 7, 419			241–243 46 93 44–47	232 22 300		0.02 aq; v s alc, eth s alc, eth s alc, bz, chl, eth
c50	4-Chlorobenzo- phenone	CIC ₆ H ₄ COC ₆ H ₅	216.67	7, 419			77	196 ^{17mm}		s alc, acet, bz, eth
c51	2-Chlorobenzotri- fluoride	CIC ₆ H ₄ CF ₃	180.56		1.3540 ²⁵	1.4513 ²⁵	-6.4	152.3		
c52	3-Chlorobenzotri- fluoride	ClC ₆ H ₄ CF ₃	180.56		1.3311 ²⁵	1.4438 ²⁵	-56.7	137.7	36	
c53	4-Chlorobenzotri- fluoride	ClC ₆ H ₄ CF ₃	180.56		1.353 ²⁰	1.4463	-33.2	138.7	47	
c54	2-(4-Chlorobenzoyl)- benzoic acid	CIC ₆ H ₄ COC ₆ H ₄ COCH	260.68	10,750			150			s alc, bz, eth
c55	2-Chlorobenzoyl	ClC ₆ H ₄ COCl	175.01	9, 336	1.382	1.5718 ²⁰	-3	238	110	d aq, alc
c56	4-Chlorobenzoyl chloride	ClC ₆ H ₄ COCl	175.01	9, 341	1.377	1.5780 ²⁰	14	222	105	d aq, alc
c57	4-Chlorobenzyl alcohol	CIC ₆ H ₄ CH ₂ OH	142.59	6, 444			72	234		v s alc, eth
c58 c59	4-Chlorobenzylamine 2-Chlorobenzyl chloride	CIC ₆ H ₄ CH ₂ NH ₂ CIC ₆ H ₄ CH ₂ Cl	141.60 161.03	12, 1074 5, 297	1.164 1.274	1.5586 ²⁰ 1.5591 ²⁰	-17	215 214	90 82	
c60	4-Chlorobenzyl chloride	CIC ₆ H ₄ CH ₂ Cl	161.03	5, 308			30	214	97	s alc; v s eth

c61	2(p-Chlorobenzyl)-	CIC ₆ H ₄ CH ₂ —C ₅ H ₄ N	203.67		1.390	1.5868 ²⁰		183 ^{20mm}	>112	
	pyridine	0 4 2 3 4								
c62	4-(<i>p</i> -Chlorobenzyl)- pyridine	CIC ₆ H ₄ CH ₂ —C ₅ H ₄ N	203.67		1.167	1.5900^{20}			>112	
c63	1-Chloro-1,3-but- adiene	H ₂ C=CHCH=CHCl	88.54	1 ³ , 949	0.9601420	1.4712^{20}		68		v s chl
c64	1-Chlorobutane	CH ₃ CH ₂ CH ₂ CH ₂ Cl	92.57	1, 118	0.8864_4^{20}	1.4021^{20}	-123.1	78.44	-6	0.11 aq; misc alc, eth
c65	2-Chlorobutane	CH ₃ CH ₂ CH(Cl)CH ₃	92.57	1, 119	0.8732420	1.3971^{20}	-113.3	68.25	-15	0.1 aq; misc alc, eth
c66	4-Chloro-1-butanol	ClCH ₂ CH ₂ CH ₂ CH ₂ OH	108.56	1 ² , 398	1.0883_4^{20}	1.4518^{20}		86-89 ^{20mm}	32	s alc, eth
c67	3-Chloro-2-butanone	CH ₃ CH(Cl)COCH ₃	106.55	1,669	1.055	1.4172^{20}		117	21	v s alc, eth
c68	cis-1-Chloro-2- butene	CH ₃ CH=CHCH ₂ Cl	90.55	1 ² , 176	0.9426_4^{20}	1.4390^{20}		84.1	-15	s alc, acet
c69	3-Chloro-1-butene	CH ₃ CH(Cl)CH=CH ₂	90.55	1 ² , 174	0.90001_4^{20}	1.4155^{20}		62-65	-20	v s acet
c70	3-Chloro-1-butyne	CH₃CH(Cl)C≡CH	88.54	1 ⁴ , 970	0.961	1.4280^{20}		68-70	1	
c71	3-Chlorobutyric acid	CH ₃ CH(Cl)CH ₂ COOH	122.55	2, 277	1.186420	1.4421^{20}	16.3	109 ^{17mm}		s alc, eth
c72	4-Chlorobutyric acid	ClCH ₂ CH ₂ CH ₂ COOH	122.55	2, 278	1.2336_4^{20}	1.4510^{20}	12-16	196 ^{22mm}	>112	sl s aq; v s eth
c73	4-Chlorobutyro- nitrile	CICH ₂ CH ₂ CH ₂ CN	103.55	2, 278	1.158	1.4413^{20}		197	85	s alc, eth
c74	4-Chlorobutyryl chloride	CICH ₂ CH ₂ CH ₂ COC1	141.00	2, 278	1.258	1.4609^{20}		174	72	d aq, alc; s eth
c75	Chloro(chloromethyl)- dimethylsilane	ClCH ₂ Si(CH ₃) ₂ Cl	143.09		1.086	1.4373^{20}		114 ^{752mm}	21	
c76	trans-p-Chloro- cinnamic acid	CIC ₆ H ₄ CH=CHCOOH	182.61	9, 594			248–250			
c77	Chlorocyclohexane	ClC ₆ H ₁₁	118.61	5, 21	1.000_4^{20}	1.4620^{20}	-44	142	28	i aq; s alc, eth
c78	2-Chlorocyclo-	$ClC_6H_9(=O)$	132.59	7, 10	1.161	1.4835^{20}	23	83 ^{10mm}	82	s bz, eth, diox
	hexanone									

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c79	Chlorocyclo-	ClC ₅ H ₉	104.58	5, 19	1.0051420	1.451220		114	15	i aq
	pentane									
c80	1-Chlorodecane	CH ₃ (CH ₂) ₉ Cl	176.73	1, 168	0.868	1.4362^{20}	-34	223	83	i aq
c81	2-Chloro-1,1-dieth- oxyethane	CICH ₂ CH(OC ₂ H ₅) ₂	152.62	1,611	1.018	1.4157^{20}		157	29	
c82	3-Chloro-1,1-dieth- oxypropane	CICH ₂ CH ₂ CH(OC ₂ H ₅) ₂	166.65	1,632	0.995	1.4240^{20}		84 ^{25mm}	36	
c83	Chlorodifluoro- acetic acid	F ₂ C(Cl)COOH	130.48	2, 201		1.3559^{20}	22.9	121.5		
c84	1-Chloro-1,1-di- fluoroethane	CH ₃ C(Cl)F ₂	100.50		1.118 ²¹		-131	-9		0.19 aq
c85	Chlorodifluoro-	HCCIF ₂	86.47		1.20921		-160	-40.8		0.30 aq
c86	methane α-Chloro-3',4'-di- hydroxyaceto-	$(HO)_2C_6H_3C(=O)CH_2CI$	186.59	8, 273			176			
	phenone									
c87	1-Chloro-2,4-di- hydroxybenzene	ClC ₆ H ₃ (OH) ₂	144.56	6 ² , 818			107	147 ^{18mm}		v s aq, alc, chl, eth
c88	2-Chloro-1,4-di- hydroxybenzene	ClC ₆ H ₃ (OH) ₂	144.56	6, 849			101–102	263		v s aq; i alc; s eth
c89	2-Chloro-1,1-di- methoxyethane	CICH ₂ CH(OCH ₃) ₂	124.57		1.094_{20}^{20}	1.4148^{20}		130	28	
c90	4-Chloro-3,5-di- methylphenol	Cl(CH ₃) ₂ C ₆ H ₂ OH	156.61	$6^2, 463$			115.5	246		0.1 aq; 1 alc; s bz, eth, alk
c91	1-Chloro-2,2-di- methylpropane	(CH ₃) ₃ CCH ₂ Cl	106.59		0.866_4^{20}	1.4042^{20}	-20	84.4		otii, aik
c92	Chlorodimethylsilane	(CH ₃) ₂ Si(Cl)H	94.62		0.852_4^{20}	1.3827^{20}	-111	36	-28	
c93	Chlorodimethylvinyl-	$(CH_3)_2Si(Cl)CH = CH_2$	120.7		0.884_4^{25}	1.414^{25}	111	82.5	-0	
	silane	(- 3/2(/2			4			-		

c94	1-Chloro-2,4-di-	ClC ₆ H ₃ (NO ₂) ₂	202.55	5, 263	1.4982475	1.585760	52–54	315	186	sl s alc; s hot alc,
0.7	nitrobenzene		202.55		4 606=16	4 505020				bz, eth
c95	1-Chloro-3,4-di-	$CIC_6H_3(NO_2)_2$	202.55	5, 262	1.686716	1.5870^{20}			>112	v s eth; s alc
-06	nitrobenzene	CIC II (NO.) COOII	246.56	0.415			100	241		0.2
c96	2-Chloro-3,5-di- nitrobenzoic acid	CIC ₆ H ₂ (NO ₂) ₂ COOH	246.56	9,415			198	241 ex-		0.3 aq
c97	α -Chlorodiphenyl-	C ₆ H ₅ CH(Cl)C ₆ H ₅	202.68	$5^2,600$	1.140_4^{20}	1.595120	17	plodes 140 ^{3mm}	>112	
097	methane	$C_6\Pi_5C\Pi(CI)C_6\Pi_5$	202.08	3,000	1.1404	1.3931	17	140	/112	
c98	Chlorodiphenyl-	$(C_6H_5)_2Si(Cl)CH_3$	232.8		1.1277_4^{20}	1.5742^{20}		295		
	methylsilane				,					
c99	Chlorodiphenyl-	$(C_6H_5)_2PCl$	220.64	16, 763	1.229	1.6338^{20}		320	>112	
	phosphine									
c100	1-Chlorododecane	CH ₃ (CH ₂) ₁₁ Cl	204.79		0.8673_4^{20}	1.4426	-9	116	93	v s alc; s bz
c101	1-Chloro-2,3-epoxy-	H ₂ Ç—ÇHCH ₂ Cl	92.53	17,6	1.1812_4^{20}	1.4381^{20}	-57.2	116.1	33	5.9 aq; misc alc,
	propane	` 0′								chl,
c102	Chloroethane	CH ₃ CH ₂ Cl	64.52	1,82	0.9214_4^0	1.3742^{10}	-136 to	12.3	-43	0.45 aq ⁰ ; 48 alc;
							-138			misc eth
c103	2-Chloroethanol	ClCH ₂ CH ₂ OH	80.52	1,337	1.197_4^{20}	1.4422^{20}	-67.5	128.6	60	misc aq, alc
c104	2-(2-Chloroethoxy)-	ClCH ₂ CH ₂ OCH ₂ CH ₂ OH	124.57	1,467	1.180	1.4529^{20}		81 ^{5mm}	90	
	ethanol							_		
c105	2-[2-(2-Chloroeth-	ClCH ₂ CH ₂ OCH ₂ CH ₂ -	168.62	1,468	1.160	1.4580^{20}		120 ^{5mm}	107	
	oxy)ethoxy]ethanol	OCH ₂ CH ₂ OH								
c106	2-Chloroethylamine	ClCH ₂ CH ₂ NH ₂ HCl	115.99	4, 133			146			
	HCl									l
c107	1-Chloro-2-ethyl-	$C1C_6H_4C_2H_5$	140.61		1.055_{25}^{25}		-81	179.2		i aq; misc alc, eth
	benzene							0.416		
c108	(2-Chloroethyl)-	C ₆ H ₅ CH ₂ CH ₂ Cl	140.61	5, 354	1.069	1.5300^{20}		84 ^{16mm}	66	s alc, bz, eth
	benzene									

Chlorodibromomethane, d71 2-Chloro-*N*,*N*-diethylethylamine, d272 Chlorodimethyl ether, c155 2-Chloro-*N*,*N*-dimethylethylamine, d467 4'-Chlorodiphenylmethanol, c44 2-Chloroethyl alcohol, c103

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c109	Chloroethylene	H,C=CHCl	62.50	1, 186	0.97^{-14}		-159.7	-13.9		sl s ag; s alc
c110	2-Chloroethyl ethyl ether	CICH ₂ CH ₂ OCH ₂ CH ₃	108.57	1, 337	0.989	1.4125 ²⁰		107	15	1.
c111	2-Chloroethyl methyl ether	CICH ₂ CH ₂ OCH ₃	94.54	1, 337	1.035	1.4111 ²⁰		89–90	15	
c112	<i>N</i> -(2-Chloroethyl)- morpholine HCl		186.08				186			
c113	N-(2-Chloroethyl)- piperidine HCl		184.11	20, 17			236			
c114	2-Chloroethyl p-toluenesulfonate	CH ₃ C ₆ H ₄ SO ₃ CH ₂ CH ₂ Cl	234.70	$11^2, 45$	1.294	1.529020		153 ^{0.3mm}	>112	
c115	2-Chloroethyl vinyl ether	H ₂ C=CHOCH ₂ CH ₂ Cl	106.55	1 ² , 473	1.048	1.4370 ²⁰	-69.7	110	16	0.6 aq
c116	1-Chloro-2-fluoro- benzene	ClC ₆ H ₄ F	130.55	5 ¹ , 110	1.244	1.5010^{20}	-42.5	138.5	31	s alc, eth
c117	1-Chloro-3-fluoro- benzene	ClC ₆ H ₄ F	130.55		1.219	1.4944 ²⁰		126	20	s alc, eth
c118	1-Chloro-4-fluoro- benzene	ClC ₆ H ₄ F	130.55	5, 201	1.226420	1.4967 ²⁰	-21.5	130–131		s alc, eth
c119	2-Chloro-6-fluoro- benzyl chloride	Cl(F)C ₆ H ₃ CH ₂ Cl	179.02		1.401	1.5372 ²⁰				
c120	4-Chloro-4'-fluoro- butyrophenone	FC ₆ H ₄ C(=O)CH ₂ CH ₂ - CH ₂ Cl	200.64		1.220	1.5255 ²⁰			110	
c121	3-Chloro-4-fluoro- nitrobenzene	Cl(F)C ₆ H ₃ NO ₂	175.5		1.602817	1.567417	41.5	127 ^{17mm}		
c122	2-Chloro-4-fluoro- phenol	Cl(F)C ₆ H ₃ OH	146.5				23	88 ^{4mm}		
c123	2-Chloro-4-fluoro- toluene	Cl(F)C ₆ H ₃ CH ₃	144.58		1.1972 ²⁰	1.4985 ²⁵		152–153		

c124	2-Chloro-6-fluoro-	Cl(F)C ₆ H ₃ CH ₃	144.58		1.191	1.5026^{20}		156	46	
	toluene									
c125	4-Chloro-2-fluoro-	Cl(F)C ₆ H ₃ CH ₃	144.58			1.4998^{20}		158		
	toluene									
c126	Chloroform	CHCl ₃	119.39	1,61	1.4985 ¹⁵	1.448615	-63.59	61.7	none	0.82 aq
c127	Chloroform-d	CDCl ₃	120.39		1.50	1.4445^{20}		60.9	none	-
c128	1-Chloroheptane	CH ₃ (CH ₂) ₆ Cl	134.65	1, 154	0.881_0^{16}	1.4250^{20}	-69	159-161	41	misc alc, eth
c129	1-Chlorohexane	CH ₃ (CH ₂) ₅ Cl	120.62		0.8780_4^{20}	1.4236^{20}		134	38	i aq
c130	6-Chloro-1-hexanol	Cl(CH ₂) ₆ OH	136.62		1.204	1.4557^{20}		108 ^{14mm}	98	sl s aq; v s alc, eth
c131	4-Chloro-4'-hydroxy-	$ClC_6H_4C(=O)C_6H_4OH$	232.67	8 ² , 187			175-178	257 ^{14mm}		
	benzophenone									
c132	5-Chloro-8-hydroxy-		305.50				d 172			i alc, eth; 0.8 chl;
	7-iodoquinoline									0.6 HOAc
c133	3-Chloro-4-hydroxy-	ClC ₆ H ₃ (OH)-	202.60				145-147			
	mandelic acid	CH(OH)COOH								
c134	5-Chloro-8-hydroxy-		179.61	21, 95			130			sl s aq HCl
	quinoline									_
c135	1-Chloro-4-iodo-	ClC ₆ H ₄ I	238.46	5, 221	1.186_4^{57}		53-54	226-227		s alc
	benzene									

2-Chloroethyl ether, b158

2-Chloro-6-fluorobenzal chloride, t233

α-Chloro-4-fluorotoluene, f16 2375-Chloro-2-hydroxyaniline, a148 Chlorohydroxybenzoic acids, c237, c238 1-Chloro-3-hydroxypropane, c214

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c136	1-Chloro-3-mercapto-	HSCH ₂ CH(OH)CH ₂ Cl	126.61	1 ³ , 2156	1.277	1.5276 ²⁰		57 ^{1.3mm}	97	
c137	2-propanol Chloromethane	CH ₃ Cl	50.49	1,59	0.92 ²⁰	1.3712^{-24}	-97.7	-24.22		0.48 aq ²⁵ ; s alc; misc chl, eth, HOAc
c137a	3-Chloro-4-methoxy-	CIC ₆ H ₃ (OCH ₃)NH ₂	157.60	13, 511			50–55			ноас
c138	5-Chloro-2-methoxy- aniline	ClC ₆ H ₃ (OCH ₃)NH ₂	157.60	13, 383			83–85			
c139	1-Chloro-2-methoxy- benzene	ClC ₆ H ₄ OCH ₃	142.59	6, 184	1.123	1.5445 ²⁰		196	76	i aq; s alc, eth
c140	1-Chloro-4-methoxy- 2-nitrobenzene	CH ₃ O(Cl)C ₆ H ₃ NO ₂	187.58				45			s hot alc
c141	2-Chloro-6-methoxy- pyridine	CH ₃ O(Cl)(C ₅ H ₃ N)	143.57		1.207	1.5263 ²⁰		186		
c142	2-Chloro-6-methyl- aniline	CH ₃ (Cl)C ₆ H ₃ NH ₂	141.60	12 ¹ , 388	1.152	1.5761 ²⁰	2	215	98	s alc
c143	3-Chloro-2-methyl- aniline	CH ₃ (Cl)C ₆ H ₃ NH ₂	141.60	12, 836		1.5874 ²⁰	2	115- 117 ^{10mm}	>112	
c144	3-Chloro-4-methyl- aniline	CH ₃ (Cl)C ₆ H ₃ NH ₂	141.60	12, 988		1.5830 ²⁰	25	238	100	
c145	4-Chloro-2-methyl- aniline	CH ₃ (Cl)C ₆ H ₃ NH ₂	141.60	12, 835		1.5848 ²⁰	27	241	99	s hot alc
c146	5-Chloro-2-methyl- aniline	CH ₃ (Cl)C ₆ H ₃ NH ₂	141.60	12, 835		1.5840 ²⁰	22	237	160	
c147	DL-4-Chloro-2-(α- methylbenzyl)- phenol	C ₆ H ₅ CH(CH ₃)- C ₆ H ₃ (Cl)OH	232.71	64,4710				155 ^{2mm}		
c148	1-Chloro-3-methyl- butane	(CH ₃) ₂ CHCH ₂ CH ₂ CI	106.59	1, 135	0.8704_4^{20}	1.4084 ²⁰	-104	99	16	sl s aq; misc alc, eth

c149	2-Chloro-2-methyl-	CH ₃ CH ₂ CCl(CH ₃) ₂	106.59	1, 134	0.8650_4^{20}	1.4052^{20}	-73.7	85	16	i aq; s alc, eth
	butane									
c150	Chloromethyldi- methylchlorosilane	(CH ₃) ₂ Si(Cl)CH ₂ Cl	143.1		1.0865_4^{20}	1.4360^{20}		115–116		
c151	Chloromethyl 2,2-di-	(CH ₃) ₃ CCOOCH ₂ Cl	150.61		1.045	1.4170^{20}			40	
C131	methylpropionate	(Cn ₃) ₃ CCOOCn ₂ CI	130.01		1.043	1.4170			40	
c152	Chloromethyl ethyl	CICH ₂ OCH ₂ CH ₃	94.54	1^2 , 645	1.04_4^{20}	1.4040^{20}		79–83		s alc; v s eth
	ether									
c153	Chloromethylmethyl-	ClCH ₂ Si(CH ₃)Cl ₂	163.5		1.2858_4^{20}	1.4500^{20}		121–122		
	dichlorosilane				20					
c154	Cloromethylmethyl-	$ClCH_2Si(OC_2H_5)_2CH_3$	182.7		1.000_4^{20}	1.407^{25}		160–161		
	diethoxysilane									
c155	Chloromethyl methyl	ClCH ₂ OCH ₃	80.51	1,580	1.0703_4^{20}	1.3961^{20}	-103.5	57–59	15	d aq; s acet, CS ₂
	ether									
c156	Chloromethyl methyl	ClCH ₂ SCH ₃	95.48		1.153	1.4963^{20}		105		
	sulfide									
c157	1-(Chloromethyl)-	$C_{10}H_7CH_2CI$	176.65	5, 566		1.6380^{20}	32	169 ^{25mm}	>112	
	naphthalene									
c158	4-Chloro-2-methyl-	$CH_3(Cl)C_6H_3OH$	142.59	6, 359			48	225		sl s aq
	phenol									
c159	4-Chloro-3-methyl-	$CH_3(Cl)C_6H_3OH$	142.59	6, 381			68	235		i aq; s alc, bz, chl,
	phenol									eth, acet
c160	4-Chloro-N-methyl-		170.08				164			
	piperidine HCl									

Chloromethylbenzenes, c244, c245, c246

(Chloromethyl)oxirane, c101

Chloromethyl pivalate, c151

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c161	1-Chloro-2-methyl- propane	(CH ₃) ₂ CHCH ₂ Cl	92.57	1, 124	0.882915	1.401015	-130.3	68.9	21	0.09 aq; misc alc, eth
c162	2-Chloro-2-methyl- propane	(CH ₃) ₃ CCl	92.57	1, 125	0.8474415	1.3856 ²⁰	-25.4	50.8	18	sl s aq; misc alc, eth
c163	1-Chloro-2-methyl- propene	(CH ₃) ₂ C=CHCl	90.55	1, 209	0.9186_4^{20}	1.4225 ²⁰		68.1	-1	misc alc, eth
c164	3-Chloro-2-methyl- propene	CICH ₂ C(CH ₃)=CH ₂	90.55	1, 209	0.9210_4^{15}	1.4272 ²⁰	-80	72	-10	misc alc, eth
c165	Chloromethyltri- chlorosilane	CICH ₂ SiCl ₃	183.9		1.465 ²⁰	1.4555 ²⁰		117–118		
c166	Chloromethyltri- methylsilane	CICH ₂ Si(CH ₃) ₃	122.7	4 ³ , 1844	0.8861_4^{20}	1.4180 ²⁰		99	<1	
c167	6-(Chloromethyl)- uracil		160.56	231, 328			257 d			
c168	1-Chloronaphthalene	C ₁₀ H ₇ Cl	162.62	5, 541	1.1938_4^{20}	1.6332^{20}	-2.3	259.3	121	s alc, bz, PE
c169	2-Chloronaphthalene	$C_{10}H_7Cl$	162.62		1.1377^{71}	1.6079^{71}	59.5	256		s alc, bz, chl, eth
c170	4-Chloro-1,8-naph- thalic anhydride		232.63	17,522			210			
c171	4'-Chloro-3'-nitro- acetophenone	$ClC_6H_3(NO_2)-$ $C(=O)CH_3$	199.60	$7^3,995$			101			
c172	2-Chloro-4-nitro- aniline	CIC ₆ H ₃ (NO ₂)NH ₂	172.57	12, 733			109			sl s aq; v s alc, eth
c172a	2-Chloro-5-nitro- aniline	ClC ₆ H ₃ (NO ₂)NH ₂	172.57	12, 732			114			
c173	4-Chloro-2-nitro- aniline	ClC ₆ H ₃ (NO ₂)NH ₂	172.57	12, 729			119			v s alc, eth
c174	4-Chloro-3-nitro- aniline	CIC ₆ H ₃ (NO ₂)NH ₂	172.57	12,731			101			v s alc; s eth

c175	1-Chloro-2-nitro- benzene	CIC ₆ H ₄ NO ₂	157.56	5, 241	1.348		32–33	246	123	s alc, bz, eth
c176	1-Chloro-3-nitro- benzene	CIC ₆ H ₄ NO ₂	157.56	5, 243	1.534 ²⁰		46	236	103	sl s alc; v s eth, chl
c177	1-Chloro-4-nitro- benzene	ClC ₆ H ₄ NO ₂	157.56	5, 243	1.520		82–84	242	110	sl s alc; v s eth, CS ₂
c178	2-Chloro-4-nitro- benzoic acid	ClC ₆ H ₃ (NO ₂)COOH	201.57	9, 404			141			s hot aq, hot bz
c179	2-Chloro-5-nitro- benzoic acid	ClC ₆ H ₃ (NO ₂)COOH	201.57	9, 403	1.60818		168			sl s aq; s alc, bz, eth
c180	4-Chloro-3-nitro- benzoic acid	ClC ₆ H ₃ (NO ₂)COOH	201.57	9, 402	1.64518		183			sl s alc; s hot aq
c181	4-Chloro-3-nitro- benzophenone	$CIC_6H_3(NO_2)-$ $C(=O)C_6H_5$	261.66	71, 230			104–105	235 ^{13mm}		
c182	2-Chloro-5-nitro- benzotrifluoride	CIC ₆ H ₃ (NO ₂)CF ₃	225.55		1.527	1.5083 ²⁰		231	98	
c183	4-Chloro-3-nitro- benzotrifluoride	CIC ₆ H ₃ (NO ₂)CF ₃	225.55		1.511	1.4893 ²⁰	-2.5	222	101	
c184	5-Chloro-2-nitro- benzotrifluoride	CIC ₆ H ₃ (NO ₂)CF ₃	225.55		1.526	1.4980 ²⁰	21–22	222–224	102	

Chloronicotinic acids, c234, c235

 α -Chloronitrotoluene, n47

Chloronitro- α , α , α -trifluorotoluenes, c182, c183, c184

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c185	o-(4-Chloro-3-nitro- benzoyl)benzoic acid	CIC ₆ H ₃ (NO ₂)COC ₆ H ₄ - COOH	305.68	10,752			201			
c186	2-Chloro-4-nitro- phenol	ClC ₆ H ₃ (NO ₂)OH	173.56	6, 240			106			
c187	2-Chloro-4-nitro- toluene	CIC ₆ H ₃ (NO ₂)CH ₃	171.58	5, 329		1.5470 ⁷⁰	61	260		i aq; s alc, eth
c188	2-Chloro-6-nitro-toluene	ClC ₆ H ₃ (NO ₂)CH ₃	171.58	5, 327		1.5377 ⁷⁰	36	238	125	i aq
c189	4-Chloro-3-nitro-toluene	ClC ₆ H ₃ (NO ₂)CH ₃	171.58	5, 329	1.297	1.5580 ²⁰	7	260 ^{745mm}	>112	i aq
c190	1-Chlorooctane	CH ₃ (CH ₂) ₇ Cl	148.68	1, 159	0.875_4^{20}	1.4298^{20}	-61	183	54	i aq; v s alc, eth
c191	1-Chloropentane	CH ₃ (CH ₂) ₄ Cl	106.60	1, 130	0.8824_4^{20}	1.4118 ²⁰	-99.0	98.3	12	0.02 aq; misc alc, eth
c192	5-Chloro-2-pentanone	CICH2CH2CH2COCH3	120.58	$1^2,738$	1.0571_4^{18}	1.4375^{20}		72 ^{20mm}	62	s acet, eth
c193	3-Chloroperoxy- benzoic acid	ClC ₆ H ₄ C(O)OOH	172.57				94 d			
c194	2-Chlorophenol	ClC ₆ H ₄ OH	128.56	6, 183	1.2573_4^{25}	1.5579^{20}	9.3	175–176	63	sl s aq; v s alc, eth
c195	3-Chlorophenol	ClC ₆ H ₄ OH	128.56	6, 185	1.245_4^{25}	1.556540	33.5	214	>112	sl s aq; s alc, eth
c196	4-Chlorophenol	ClC ₆ H ₄ OH	128.56	6, 186	1.2238478	1.541945	43.5	220	115	sl s aq; v s alc, chl, eth
c197	4-Chlorophenoxy- acetic acid	ClC ₆ H ₄ OCH ₂ COOH	186.59	6, 187			159			
c198	2-(4-Chlorophenoxy)- 2-methylpropionic acid	CIC ₆ H ₄ OC(CH ₃) ₂ COOH	214.65				122			
c199	DL-2-(4-Chlorophenoxy)propionic acid	CIC ₆ H ₄ OCH(CH ₃)COOH	200.62	$6^3,695$			117			

c200	4-Chlorophenylacetic	CIC ₆ H ₄ CH ₂ COOH	170.60	9,448			105			v s aq, alc, eth; s
	acid									bz
c201	<i>p</i> -Chlorophenylaceto- nitrile	ClC ₆ H ₄ CH ₂ CN	151.60	9,448			30.5	267		
c202	2-Chloro- <i>p</i> -phenyl- enediamine sulfate	H ₂ NC ₆ H ₃ (Cl)NH ₂ · H ₂ SO ₄	240.67	13, 117			253			
c202	4-Chloro-1,2-phenyl- enediamine	$ClC_6H_3(NH_2)_2$	142.59	13, 25			70			
c204	4-Chloro-1,3-phenyl- enediamine	H ₂ N(Cl)C ₆ H ₃ NH ₂	142.59	13, 53			90			
c205	3-Chlorophenyl- hydrazine HCl	ClC ₆ H ₄ NHNH ₂ ·HCl	179.05	15, 424			242 d			
c206	4-Chlorophenyl isocyanate	ClC ₆ H ₄ NCO	153.57	12,616		1.5618 ²⁰	31	204	110	
c207	4-Chlorophenyl phenyl sulfone	ClC ₆ H ₄ SO ₂ C ₆ H ₅	252.72	6 ¹ , 149			94			74 acet; 44 bz; 5 CCl ₄ ; 65 diox; 21 i-PrOH
c208	4-Chlorophenyltri- chlorosilane	ClC ₆ H ₄ SiCl ₃	246.0		1.4316420	1.5418 ²⁰		115- 117 ^{20mm}		211-FIOH
c209	4-Chloro- <i>o</i> -phthalic acid	CIC ₆ H ₃ (COOH) ₂	200.58	9,816			148			
c210	1-Chloropropane	CH ₃ CH ₂ CH ₂ Cl	78.54	1, 104	0.898515	1.3880^{20}	-122.8	46.6	18	0.27 aq; misc alc,
c211	2-Chloropropane	CH ₃ CHClCH ₃	78.54	1, 105	0.8563^{20}	1.3777^{20}	-117.2	35	-35	0.34 aq; misc alc,
c212	3-Chloro-1,2- propanediol	ClCH ₂ CH(OH)CH ₂ OH	110.54		1.3218420	1.4805^{20}		213	58	s aq, alc, eth
c213 c214	1-Chloro-2-propanol 3-Chloro-1-propanol	CH ₃ CH(OH)CH ₂ Cl ClCH ₂ CH ₂ CH ₂ OH	94.54 94.54	1, 363 1, 356	$\begin{vmatrix} 1.115^{20} \\ 1.1309_4^{20} \end{vmatrix}$	$1.4375^{20} 1.4460^{20}$		126–127 160–162	51 73	misc aq; s alc

p-Chlorophenacyl bromide, b246 Chlorophenylamines, c33, c34, c35 4-Chlorophenyl sulfone, b165 4-Chlorophenyl sulfoxide, b166 Chloropicrin, t239 Chloroprene, c216

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c215	Chloro-2-propanone	CICH ₂ COCH ₃	92.53	1,653	1.13545	1.4350 ²⁰	-44.5	119.7	7	10 aq; misc alc,
c216	3-Chloro-1-propene	CICH ₂ CH=CH ₂	76.53	1, 198	0.939420	1.4151^{20}	-134.5	45.2	-28	0.36 aq; misc alc,
c217	(3-Chloropropenyl)- benzene	C ₆ H ₅ CH=CHCH ₂ Cl	152.62	5 ² , 372		1.5845 ²⁰	-19	108 ^{12mm}	79	CIII
c218	2-Chloropropionic acid	CH ₃ CH(Cl)COOH	108.52	2, 248	1.182	1.4345^{20}		186	101	misc aq, alc, eth
c219	3-Chloropropionic acid	CICH ₂ CH ₂ COOH	108.52	2, 249			41	205	>112	v s aq, alc, chl
c220	3-Chloropropio- nitrile	CICH ₂ CH ₂ CN	89.53	2, 250	1.144318	1.4379^{20}	-50	176	75	
c221	2-Chloropropionyl chloride	CH ₃ CH(Cl)COCl	126.97	2, 248	1.308	1.4400^{20}		111	31	d aq, alc
c222	3-Chloropropionyl chloride	CICH ₂ CH ₂ COCl	126.97	2, 250	1.330713	1.4570^{20}		145	61	i aq; d hot aq, hot alc; s alc; v s eth
c223	p-Chloropropio- phenone	$CIC_6H_4C(=O)CH_2CH_3$	168.62	7, 301			37	97 ^{1mm}		
c224	3-Chloropropylamine HCl	CICH ₂ CH ₂ CH ₂ NH ₂ ·HCl	130.02	4, 148			150			
c225	3-Chloropropyl- methyldichloro- silane	Cl(CH ₂) ₃ Si(CH ₃)Cl ₂	191.6		1.2045 ₄ ²⁰	1.4580 ²⁰		70 ^{15mm}		
c226	2-Chloropropyl- (phenyl)dichloro- silane	Cl(CH ₂) ₃ SiCl ₂ (C ₆ H ₅)	253.6		1.241420	1.5332 ²⁰		141 ^{10mm}		
c227	N-(3-Chloropropyl)- piperidine HCl		198.14	20, 18			220			

c228	3-Chloropropyl	CH ₃ C(=O)SCH ₂ CH ₂ CH ₂ Cl	152.64	$2^3,493$	1.159	1.4946^{20}		84 ^{10mm}	77	
c229	thiolacetate 3-Chloropropyltri- chlorosilane	CICH ₂ CH ₂ CH ₂ SiCl ₃	212.0		1.3590420	1.4668 ²⁰		181.5	66	
c229	3-Chloropropyltri- ethoxysilane	Cl(CH ₂) ₃ Si(OC ₂ H ₅) ₃	240.8	1.009_4^{20}	1.42020			102 ^{10mm}		
c231	3-Chloropropyltri- methoxysilane	Cl(CH ₂) ₃ Si(OCH ₃) ₃	198.72		1.077_4^{25}	1.4183 ²⁵		183	66	
c232	3-Chloropropyne	ClCH ₂ C≡CH	74.51	1, 248	1.0306425	1.4349^{20}	-78	58	18	misc bz, alc, eth, EtAc
c233	2-Chloropyridine	ClC₅H₄N	113.55	20, 230	1.20515	1.5320^{20}		166 ^{714mm}	65	sl s aq; s alc, eth
c234	2-Chloro-3-pyridine- carboxylic acid	C ₅ H ₃ N(Cl)COOH	157.56	22 ² , 35			d 175			
c235	6-Chloro-3-pyridine- carboxylic acid	C₅H₃N(Cl)COOH	157.56	22, 43			200 d			
c236	2-Chloroquinoline		163.61	20, 359	1.2464_4^{25}	1.6259^{25}	37	267		i aq; s alc, bz, eth
c237	4-Chlorosalicyclic acid	HO(Cl)C ₆ H ₃ COOH	172.57	10, 101			212			
c238	5-Chlorosalicylic acid	HO(Cl)C ₆ H ₃ COOH	172.57	10, 102			172			
c239	N-Chlorosuccinimide		133.53	21, 380	1.65		150–151			1.4 aq; 0.67 alc; 2 bz; sl s chl, eth
c240	Chlorosulfonyl isocyanate	CISO ₂ NCO	141.53		1.626	1.4467^{20}	-44	107		

 β -Chloropropionaldehyde diethyl acetal, c82

3-Chloropropylene-1,2-oxide, c102

1-Chloro-2,5-pyrrolidinedione, c239

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c241	8-Chlorotheophylline		214.61	26, 473			d 290			s alk
c242	2-Chlorothiophene	Cl—C ₄ H ₃ S	118.59	17, 32	1.286	1.5483^{20}	-72	129	22	i aq; misc alc, eth
c243	4-Chlorothiophenol	ClC ₆ H ₄ SH	144.62	6, 326			51	207		
c244	2-Chlorotoluene	ClC ₆ H ₄ CH ₃	126.59	5, 290	1.0826_4^{20}	1.5250^2	-34	159.0	47	sl s aq; v s alc, bz, chl, eth
c245	3-Chlorotoluene	CIC ₆ H ₄ CH ₃	126.59	5, 291	1.076019	1.521820	-48.9	161.8	50	s alc, bz, chl; misc
0243	3-Cinorototuche	CIC ₆ II ₄ CII ₃	120.39	3, 291	1.07004	1.5216	40.9	101.6	30	eth
c246	4-Chlorotoluene	ClC ₆ H ₄ CH ₃	126.59	5, 292	1.0697 ₄ ²⁰	1.5208 ²⁰	7.2	162.0	49	sl s aq; s alc, bz, eth
c247	N-Chloro-p-toluene- sulfonamide, Na salt	CH ₃ C ₆ H ₄ SO ₂ NCl ⁻ Na ⁺	227.67				167 d			s aq; i bz, chl, eth
c248	4'-Chloro-1- toluenethiol	ClC ₆ H ₄ CH ₂ SH	158.65	6, 466	1.202	1.5893 ²⁰	20		76	
c249	4-Chloro- <i>o</i> -tolyloxy- acetic acid, Na salt	CIC ₆ H ₃ (CH ₃)O- CH ₂ COO ⁻ Na ⁺	222.61	6 ³ , 1265			220–225			
c250	4-(4-Chloro- <i>o</i> -tolyl-oxy)butyric acid	CIC ₆ H ₃ (CH ₃)O- (CH ₂) ₃ COOH	228.68				99–100			
c251	Chloro-2,2,2-tri- fluoroethane	CF ₃ CH ₂ Cl	118.5		1.3890	1.3090°	-105	6.9		
c252	Chlorotrifluoro- ethylene	CF ₂ =CFCl	116.48		1.315		-158.2	-27.9		
c253	Chlorotrifluoro- methane	CICF ₃	104.46	1 ³ , 42			-181	-81.5		
c254	Chlorotrimethyl-	(CH ₃) ₃ GeCl	153.16		1.238222	1.4283^{20}	-13	102		
	germane									
c255	Chlorotrimethyl-	(CH ₃) ₃ SiCl	108.64		0.8580_4^{20}	1.3885^{20}	-40	57	-40	
	silane									

c256	Chlorotriphenyl-	$(C_6H_5)_3CC1$	278.78	5,700			110–112	230 ^{20mm}		v s bz, chl, eth
c257	methane Chlorotripropyl-	$(C_3H_7)_3SiCl$	192.8		0.882_4^{20}	1.440^{20}		199–201		
C231	silane	(C ₃ 11 ₇) ₃ 51C1	192.0		0.8824	1.440		199-201		
c257a	Chlorotris(di-	[(CH ₃) ₂ N] ₃ SiCl	195.8		0.975_4^{20}	1.442^{20}		62-63 ^{12mm}		
	methylamino)silane									
c258	α -Chloro- o -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 364	1.063	1.5391^{20}		199	73	i aq; misc alc, eth
c259	α -Chloro- m -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 373	1.064^{20}	1.5350^{20}		195-196	75	i aq; misc alc, eth
c260	α -Chloro- p -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 384		1.5330^{20}	4.5	200	75	misc alc, bz, eth,
										acet
c261	4-Chloro-o-xylene	$ClC_6H_3(CH_3)_2$	140.61	5, 363	1.047	1.5283^{20}		223	66	misc alc, bz, eth,
										acet
c262	Cholesterol		386.66		1.067_4^{20}		148.5	360 sl d		1.29 alc; 35 eth; 22
										chl; s bz, PE
c263	Cholic acid		408.58				198			0.028 aq; 0.06 alc;
										2.8 acet; 0.036
							1			bz; 0.5 chl

α-Chlorotoluene, b89 Chlorotoluidines, c142, c143, c144, c145, c146 2-Chlorotriethylamine, d272 Chloro- α , α , α -trifluorotoluenes, c51, c52, c53 4-Chloro- α , α , α -trifluoro-o-toluidine, a144 α' -Chloro- α , α , α -trifluoro-m-xylene, t299 Chlorotrihexylsilane, t302 Chloroxylenol, c90

CH₃

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c264	Cinchonine		294.40	23 ² , 369			~260			1.4 alc; 0.9 chl; 0.2
					25					eth
c265	1,8-Cineole		154.25	17, 23	0.921_{25}^{25}	1.457220	1.5	174.4		misc alc, chl, eth
c266	trans-Cinnam- aldehyde	C ₆ H ₅ CH=CHCHO	132.16	7, 348	1.050_{25}^{25}	1.621920	-7.5	246	71	0.014 aq; misc alc, chl, eth
c267	trans-Cinnamic acid	C ₆ H ₅ CH=CHCOOH	148.16	9, 573	1.24754		134	300		0.05 aq; 16 alc; 8
c268	trans-Cinnamoyl	C ₆ H ₅ CH=CHCOCl	166.61	9 ² , 390	1.1617_4^{25}	1.614 ⁴³	35–36	258		s hot alc, CCl ₄
c269	Cinnamyl alcohol	C ₆ H ₅ CH=CHCH ₂ OH	134.18	6,570	1.039735	1.5758 ³³	33	250.0		s ag; v s alc, eth
c270	Citraconic acid	CH ₃ C(COOH)=CHCOOH	130.10	2, 768	1.62	1.0700	92 d	200.0		v s aq, alc, eth; sl
02.0			150110	2,700	11.02		/24			s chl; i bz, PE
c271	Citraconic anhydride		112.08	17, 440	1.247	1.4712^{20}	8	214	101	
c272	Citrazinic acid		155.11	22, 254			car-			i aq; s alk
							bonizes			
							with-			
							out			
							melt-			
							ing			
							>300			
c273	Citric acid	HOOCCH ₂ C(OH)(COOH)-	192.12	3,556	1.665		154			59 aq
27.4	G'. 11 1	CH ₂ COOH	156.05	1 451	0.057020	1 455620		222	70	
c274	Citronellol	(CH ₃) ₂ C=CHCH ₂ CH ₂ CH-	156.27	1,451	0.8570_4^{20}	1.4556 ²⁰		222	79	
c275	Cocaine	(CH ₃)CH ₂ CH ₂ OH	303.35	22 ² , 150		1.502298	98	187 ^{0.1mm}		0.17 aq; 15 alc;
6213	Cocame		303.33	22,130		1.3022	96	107		140 chl; 28 eth
c276	Coumarin		146.15	17, 328	0.935_4^{20}		69	298		0.25 aq; v s alc,
										chl, eth
	•	'		'						•

c277	Creatine	$HOOCCH_2N(CH_3)-$ $C(=NH)NH_2$	131.14	4, 363			300			1.3 aq; 0.11 alc; ith
c278	Creatinine	2 (2 122)2 1222	113.12	24, 245			255 d			8 ag; sl s alc; i eth
c279	o-Cresol	CH ₃ C ₆ H ₄ OH	108.14	6, 349	1.027341	1.536141	30.9	190.8	81	3.1 aq ⁴⁰ ; misc alc, chl, eth; s alk
c280	m-Cresol	CH ₃ C ₆ H ₄ OH	108.14	6, 373	1.034420	1.543820	12.2	202.7	86	2.5 aq ⁴⁰ ; misc alc, chl, eth; s alk
c281	p-Cresol	CH₃C ₆ H₄OH	108.14	6, 389	1.017941	1.531241	34.8	201.9	86	2.3 aq ⁴⁰ ; misc alc, chl, eth; s alk
c282	trans-Crotonaldehyde	CH₃CH=CHCHO	70.09	1,728	0.8516^{20}	1.4373^{20}	-76.5	104.1	8	18.1 aq
c283	Crotonyl chloride	CH ₃ CH=CHCOCl	104.54	2,411	1.091	1.4595^{20}		123	35	_
c284	Cupferron	$C_6H_5N(NO)O^-NH_4^+$	155.16	16 ¹ , 395			163-164			v s aq, alc

Chromone, b56 Chromotropic acid, d396 Chrysoldin, d31 Cinchophen, p149 Cinnamyl chloride, c217 Citral, d562, d563 Cleland's reagent, d424 2,4,6-Collidine, t367 p-Coumaric acid, h107 Cresotic acids, h137, h138 Cresylic acids, c279, c280, c281 Crotonic acid, b402 Crotononitrile, b400 Crotyl alcohols, b404, b405 Crotyl bromide, b240 Crotyl chloride, c68 12-Crown-4, t125 15-Crown-5, p45 18-Crown-6, h74 Cumene, i91 Cumic alcohol, i92 Cupron, b50

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c285	Cyanamide	H ₂ NCN	42.04	3 ² , 63	1.282420		46	83 ^{380mm}		78 aq; 29 BuOH; 42 EtAc; s alc, eth
c286	2-Cyanoacetamide	NCCH ₂ CONH ₂	84.08	2, 589			119.5		215	25 aq; 3.1 alc
c287	Cyanoacetic acid	NCCH ₂ COOH	85.06	2, 583			65–67	108 ^{15mm}	107	s aq, alc, eth; sl s bz
c288	Cyanoacetohydrazide	NCCH ₂ C(=O)NHNH ₂	99.09				110	d		v s aq; s alc; i eth
c289	Cyanoacetylurea	NCCH ₂ C(=0)NHC(=0)- NH ₂	127.10	3, 66			214 d			
c290	2-Cyanoethanol	NCCH ₂ CH ₂ OH	71.08	$3^2, 213$	1.05880			106- 108 ^{11mm}		misc aq, alc; sl s eth
c291	2-Cyanoethyldi- chloromethylsilane	NCCH ₂ CH ₂ Si(CH ₃)Cl ₂	168.1		1.202_4^{20}	1.455 ²⁰		63 ^{4mm}		
c292	1-Cyano-3-methyliso- thiourea, Na salt	CH ₃ NHC(=NCN)S ⁻ Na ⁺	137.14	4,71			290 d			
c293	1-Cyanonaphthalene	C ₁₀ H ₇ CN	153.18	9, 649	1.1113_{25}^{25}	1.629818	38	299		i aq; v s alc, eth
c293	3-Cyanopropyltri- chlorosilane	NCCH ₂ CH ₂ CH ₂ SiCl ₃	202.6		1.280 ²⁵	1.465 ²⁵		93– 94 ^{8mm}		
c295	2-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 36		1.5288 ²⁰	28	215	89	s aq; v s alc, bz, eth
c296	3-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 41			52	240-245		v s aq, alc, bz, eth
c297	4-Cyanopyridine	$NC(C_5H_4N)$	104.11	22, 46			80			s aq, alc, bz, eth
c298	Cyanotrimethylsilane	(CH ₃) ₃ SiCN	99.21		0.783_4^{20}	1.3924^{20}	11	114–117	1	
c299	Cyanuric acid		129.08	26, 239	1.7680		d to HO- CN			0.5 aq; s hot alc, pyr; i acet, bz, chl, eth
c300	Cyclobutane	C_4H_8	56.10	5, 17	0.7038°	1.3752°	-90.7	12.5		i aq; v s alc, acet
c301	Cyclodecane	$C_{10}H_{20}$	140.27			1.4707^{20}		201	1	
c302	Cyclododecanol	$C_{12}H_{23}OH$	184.32				77			

c303 c304	Cyclododecanone trans,trans,cis- 1,5,9-cyclododeca-	$C_{12}H_{22}(=0)$	182.31 162.28	$7^2, 48$	$\begin{bmatrix} 0.906 \\ 0.8925_4^{20} \end{bmatrix}$	1.5070^{20}	61 -18	85 ^{1mm} 231	87	
	triene									
c305	trans-Cyclododecene		166.31		0.863	1.4822^{20}		232–245	93	
c306	Cycloheptane	C_7H_{14}	98.18	5, 29	0.811_4^{20}	1.4455^{20}	-8.0	118.8	6	v s alc, eth
c307	DL-trans-1,2-	$C_7H_{12}(OH)_2$	130.19	$6^3,4086$			61-63	138-		
	Cycloheptanediol							139 ^{15mm}		
c308	Cycloheptanol	$C_7H_{13}OH$	114.19	6, 10	0.948_4^{20}	1.4760^{20}	2	185	71	sl s aq; v s alc, eth
c309	Cycloheptanone	$C_7H_{12}(=0)$	112.17	7, 13	0.9490_4^{20}	1.4611^{20}		179-181	55	i aq; v s alc; s eth
c310	1,3,5-Cyclohepta-		92.13	5, 280	0.888	1.5211^{20}	-75.3	115.5	26	s alc, eth; v s bz,
	triene									chl
c311	Cycloheptene	C_7H_{12}	96.17	5, 65	0.824_4^{20}	1.4585^{20}		114.7	-6	s alc, eth
c312	Cyclohexane	C_6H_{12}	84.16	5, 20	0.7786_4^{20}	1.4262^{20}	6.5	80.7	-18	0.01 aq; misc alc,
										bz, acet, eth,
										CCl ₄
c313	Cyclohexane-d ₁₂	C_6D_{12}	92.26		0.89	1.4210^{20}		78	-18	

Cyanoacetonitrile, m5 Cyanoanilines, a124, a125, a126 Cyanobenzene, b51 2-Cyanoethanol, h169 Cyanoethylene, a64 Cyanomethane, a29 2-Cyanopropene, m27 Cyanuric chloride, t250 Cyclododecane epoxide, e4 Cyclododecanone isooxime, a318 Cycloheptanone isooxime, a317 Cycloheptyl bromide, b260 Cyclohexaneacetic acid, c333 Cyclohexanecarboxylic acid chloride, c316 2,5-Cyclohexadien-1,4-dione, b59 2,5-Cyclohexadiene-1,4-dione with 1,4benzenediol (1:1), q1 Cyclohexanemethanol, c342









TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c314	1,3-Cyclohexanebis-	C ₆ H ₁₀ (NHCH ₃) ₂	142.25						106	
c315	(methylamine) Cyclohexanecarb- aldehyde	C ₆ H ₁₁ CHO	112.17	7, 19	0.926	1.4500 ²⁰		163	40	
c316	Cyclohexanecarbonyl chloride	C ₆ H ₁₁ COCl	146.62	9,9	1.096	1.4700 ²⁰		184	66	
c317	Cyclohexanecar- boxylic acid	C ₆ H ₁₁ COOH	128.17	7, 19	1.0480415	1.4530 ²⁰	29	232.5		0.21 aq; s alc, bz, eth
c318	cis-1,2-Cyclohex- anediamine	$C_6H_{10}(NH_2)_2$	114.19	13, 1	0.931	1.4864 ²⁰		92 ^{18mm}		
c319	trans-1,2-Cyclohex- anediamine	$C_6H_{10}(NH_2)_2$	114.19	13, 1	0.931	1.4864 ²⁰		92 ^{18mm}		
c320	cis-1,2-Cyclohexane- dicarboxylic anhydride		154.17				34	158 ^{17mm}		
c320	cis-1,4-Cyclohexane- dimethanol	C ₆ H ₁₀ (CH ₂ OH) ₂	144.21		0.9784100	1.4893 ²⁰ super- cooled	43	288	74	misc aq, alc; 2.5 eth
c322	1,3-Cyclohexanedione	$C_6H_8(=0)$	112.13	7, 554	1.086191	1.4576102	103–105			s aq, alc, acet, chl
c323	1,2-Cyclohexanedione	$C_6H_8(=NOH)_2$	142.16	17 ² , 526			185–188			s aq
c324	Cyclohexanemethyl- amine	$C_6H_{11}CH_2NH_2$	113.20	12, 12	0.870	1.4630 ²⁰		145–147	43	
c325	Cyclohexanepropionic acid	C ₆ H ₁₁ CH ₂ CH ₂ COOH	156.23	9, 82	0.912	1.4636 ²⁰	14–17	275.8		
c326	Cyclohexanethiol	C ₆ H ₁₁ SH	116.23	6, 8	0.950	1.4921^{20}		158-160	43	
c327	Cyclohexanol	C ₆ H ₁₁ OH	100.16	6, 5	0.9416 ³⁰	1.462930	25.2	161.1	67	3.8 aq ²⁵ ; misc alc, bz

c328	Cyclohexanone	$C_6H_{10}(=0)$	98.15	7,8	0.9478_4^{20}	1.4510^{20}	-45 to	155.7	46	15 aq ¹⁰ ; s alc, eth
c329	Cyclohexanone oxime	$C_6H_{10}(=NOH)$	113.16	7, 10	2000 120		-47 89-91	206–210		s aq, eth; sl s alc
c330	Cyclohexene	C_6H_{10}	82.15	5, 63	0.8094_4^{20}	1.4464 ²⁰	-103.5	83.0	-12	0.02 aq; misc alc, bz, acet, eth
c331 c332	2-Cyclohexen-1-one 2,3-Cyclohexeneo- pyridine	$C_6H_8(=O)$	96.13 133.19	7 ² , 55 20 ² , 176	0.993 1.025	1.4885 ²⁰ 1.5440	-53	168 218	61 86	v s alc
c332a	[2-(3-Cyclohexenyl)- ethyl]methyldi- chlorosilane	C ₆ H ₉ CH ₂ CH ₂ Si (CH ₃)Cl ₂	223.2		1.0774	1.481 ²⁵		79–81 ^{2mm}		
c333	Cyclohexylacetic acid	C ₆ H ₁₁ CH ₂ COOH	142.20	$9^2, 9$	1.007	1.4630 ²⁰	31–33	242–244	>112	sl s aq; s org solv
c334	Cyclohexylamine	$C_6H_{11}NH_2$	99.18	12, 5	0.8671 ²⁰	1.4593 ²⁰	-17.7	134.8	<32	misc aq, alc, eth,
c335	2-(Cyclohexylamino)- ethanesulfonic acid	C ₆ H ₁₁ NHCH ₂ CH ₂ SO ₃ H	207.29				>300			
c336	3-Cyclohexylamino-1- propanesulfonic acid	C ₆ H ₁₁ NHCH ₂ CH ₂ - CH ₂ SO ₃ H	221.32				>300			

Cyclohexanone cyanohydrin, h110 cis-4-Cyclohexene-1,2-dicarboximide, t75 cis-4-Cyclohexene-1,2-dicarboxylic anhydride, t74 Cyclohexene oxide, e5 *N*-(1-Cyclohexen-1-yl)morpholine, m450 *N*-(1-Cyclohexen-1-yl)pyrrolidine, p274

Cyclohexyl alcohol, c327

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c337 c338	4-Cyclohexylaniline Cyclohexylbenzene	C ₆ H ₁₁ C ₆ H ₄ NH ₂ C ₆ H ₁₁ C ₆ H ₅	175.28 160.26	12, 1209 5, 503	0.9502420	1.5258 ²⁰	53–56 5–6	166 ^{13mm} 239–240	98	i aq; v s alc, eth
c339	N-Cyclohexylform- amide	C ₆ H ₁₁ NHCHO	127.18				38–40	137 ^{10mm}		
c340	Cyclohexyl isocyanate	C ₆ H ₁₁ NCO	125.17	12 ² , 12	0.980	1.4551^{20}		168–170	48	
c341	Cyclohexyl isothiocyanate	C ₆ H ₁₁ NCS	141.24	12 ² , 12	0.996	1.5350^{20}		219		
c342	Cyclohexylmethanol	C ₆ H ₁₁ CH ₂ OH	114.19	6, 14	0.9512_4^{25}	1.4640^{25}		181	71	s alc, eth
c343	N-Cyclohexyl-2- pyrrolidinone		167.25		1.026	1.495	12	284		
c344	Cyclohexyltrichloro- silane	C ₆ H ₁₁ SiCl ₃	217.6		1.222_4^{20}	1.477^{20}		90– 91 ^{10mm}		
c345	1,5-Cyclooctadiene		108.18	5, 116	0.8818_4^{25}	1.4905^{25}	-69	149-150	45	s CCl ₄
c346	Cyclooctane	C_8H_{16}	112.22	5, 35	0.834	1.4574^{20}	14.8	151.1	30	
c347	Cyclooctanol	C ₈ H ₁₅ OH	128.22	$6^2, 25$	0.9740_4^{20}	1.4850^{20}	14–15	106- 108 ^{22mm}	86	
c348	Cyclooctanone	$C_6H_{14}(=0)$	126.20	7, 21	0.9584_4^{20}	1.6494^{20}	41-43	195–197		
c349	Cyclooctene	C_8H_{14}	110.20	$5^1, 35$	0.846	1.4698^{20}	-16	145–146	25	
c350	Cyclooctylamine	$C_8H_{15}NH_2$	127.23		0.928	1.4804^{20}	-48	190	62	
c351	Cyclopentamethylene- dichlorosilane		169.1		1.558 ²⁰	1.4679 ²⁰		169–170		
c352	Cyclopentane	C_5H_{10}	70.13	5, 19	0.7460_4^{20}	1.4065^{20}	-93.9	49.3	-37	i aq; misc alc, eth
c353	Cyclopentanecarb- oxylic acid	C ₅ H ₉ COOH	114.14	9, 6	1.053 ²⁰	1.4540^{20}	4	216	93	sl s aq; s MeOH
c354	cis,cis,cis,cis-1,2,3,4-	$C_5H_6(COOH)_4$	246.17	$9^2,724$			192-			
	Cyclopentane-						195 d			
	tetracarboxylic									
	acid									

c355	Cyclopentanol	C_5H_0OH	86.13	6,5	0.948840	1.4521^{20}	-19	140.9	51	sl s aq; s alc
c356	Cyclopentanone	$C_5H_8(=0)$	84.12	7,5	0.9509_4^{18}	1.4366 ²⁰	-58	130.6	30	sl s aq; misc alc, eth
c357	Cyclopentanone oxime	$C_5H_8(=NOH)$	99.13	7,7			53–55	196		s aq, alc, bz, chl, eth
c358	Cyclopentene	C_5H_8	68.11	5, 61	0.774	1.4228^{20}	-135.1	44.2	-28	
c359	2-Cyclopentene-1- acetic acid	C ₅ H ₇ CH ₂ COOH	126.16	9, 42	1.047	1.4675^{20}	19	93- 94 ^{2.5mm}	>112	
c360	2,3-Cyclopenteneo- pyridine		119.17		1.018	1.5445 ²⁰		87- 88 ^{11mm}	67	
c361	N-(1-Cyclopentene-1-yl)morpholine		153.23		0.957	1.5105^{20}		105- 106 ^{12mm}	60	
c362	2-Cyclopentylidene- cyclopentanone		150.22		1.001	1.5231 ²⁰		140 ^{20mm}	103	
c363	3-Cyclopentylpro- pionic acid	C ₅ H ₉ CH ₂ CH ₂ COOH	142.20		0.996	1.4570^{20}		130 ^{12mm}	46	
c364	Cyclopropane	C_3H_6	42.08	5, 15	0.720_4^{-79}		-127.4	-32.8		37 mL per 100 mL aq ¹⁵ ; v s alc, eth

Cyclohexylbenzene, p104 Cyclohexyl bromide, b261 Cyclohexyl chloride, c77 Cyclohexyl ketone, c328 Cyclohexyl mercaptan, c326 Cyclohexylmethane, m194 Cyclohexylmethyl bromide, b306 Cyclooctene oxide, e7a Cyclopentanepropanoic acid, c363 Cyclopentene oxide, e37 Cyclopentyl bromide, b263 Cyclopentyl chloride, c79 Cyclopropyl bromide, b264 Cyclopropyl cyanide, c365

c343

c345

c351

c360

c361

c362

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c365	Cyclopropanecarbo- nitrile	C ₃ H ₅ CN	67.09	9, 4	0.91116	1.420720		135	32	s eth
c366	Cyclopropane- carbonyl chloride	C ₃ H ₅ COCl	104.54	9, 4	1.152	1.4522 ²⁰		119	23	
c367	Cyclopropanecarb- oxylic acid	C₃H₅COOH	86.09	9, 4	1.008	1.4380 ²⁰	17–19	182–184	71	sl s hot aq; s alc, eth
c368	Cyclopropyl methyl ketone	C ₃ H ₅ COCH ₃	84.12	7,7	0.8993_4^{20}	1.4241 ²⁰		114	21	s aq, alc, eth
c369	Cystamine dihydro- chloride	H ₂ NCH ₂ CH ₂ SSCH ₂ - CH ₂ NH ₂ ·2HCl	225.20	4, 287			217 d			
c370	L-(+)-Cysteine	HSCH ₂ CH(NH ₂)COOH	121.16	4, 506			220 d			v s aq, alc; i bz, eth
c371	L-Cystine	HOOCCH(NH ₂)CH ₂ - SSCH ₂ CH(NH ₂)COOH	240.30	4, 507			d 240			0.01 aq; s acid, alk; i alc
d1	cis-Decahydronaph- thalene	$C_{10}H_{18}$	138.26	5,92	0.8963420	1.4810 ²⁰	-43.0	195.8	58	v s alc, chl, eth; misc most ketones, esters
d2	trans-Decahydro- naphthalene	$C_{10}H_{18}$	138.26	$5^2, 56$	0.8700_4^{20}	1.4697 ²⁰	-30.4	187.3	52	see under <i>cis</i> isomer
d3	Dehydro-2-naphthol	C ₁₀ H ₁₇ OH	154.25	6, 67	0.996	1.4992		109 ^{14mm}	>112	
d4	Decamethylcyclo- pentasiloxane	$[-Si(CH_3)_2O-]_5$	370.8		0.959_4^{20}	1.398220	-38	101 ^{20mm}		i aq
d5	Decamethyltetra- siloxane	(CH ₃) ₃ SiO[Si(CH ₃) ₂ O] ₂ - Si(CH ₃) ₃	310.7		0.8536_4^{20}	1.3880 ²⁰	-70	194–195	86	sl s alc; s bz, PE
d6	Decanal	H(CH ₂) ₉ CHO	156.27	1,711	0.830_4^{15}	1.4280^{20}		207-209	85	i aq; s alc, eth
d7	Decane	CH ₃ (CH ₂) ₈ CH ₃	142.29	1, 168	0.7301_4^{20}	1.4119^{20}	-29.7	174.1	46	0.07 aq
d8	1,10-Decanediamine	$H_2N(CH_2)_{10}NH_2$	172.32	4, 273			62-63	140 ^{12mm}		_
d9	Decanedioic acid	HOOC(CH ₂) ₈ COOH	202.25	2,718	1.207_4^{20}	1.422134	134.5	295 ^{100mm}		0.1 aq; v s alc, esters, ketones
d10	1,10-Decanediol	HO(CH ₂) ₁₀ OH	174.28	$1^2,560$			72–75	170 ^{8mm}		sl s aq, eth; v s alc

d11	Decanedioyl dichloride	ClC(O)(CH ₂) ₈ COCl	239.14	2,719	1.1212_4^{20}	1.4678^{20}		220 ^{75mm}	>112	d aq, alc
d12	Decanenitrile	CH ₃ (CH ₂) ₈ CN	153.27	2,356	0.8295_4^{15}	1.4295^{20}	-15	235–237		misc alc, chl, eth
d13	1-Decanesulfonic acid, Na salt	CH ₃ (CH ₂) ₉ SO ₃ ⁻ Na ⁺	244.33	$4^3, 27$	0.02,04		300			
d14	Decanoic acid	CH ₃ (CH ₂) ₈ COOH	172.27	$2^2,309$	0.8782_4^{50}	1.4288^{40}	31.4	270		0.015 aq; s alc, chl, bz, eth, CS ₂
d15	1-Decanol	CH ₃ (CH ₂) ₀ OH	158.29	1, 425	0.8297_4^{20}	1.4371^{20}	6.9	230.2	82	i aq; s alc, eth
d16	4-Decanone	$CH_3(CH_2)_5C(=O)$ - $(CH_2)_5CH_3$	156.27	1,711	0.824_0^{20}	1.4237^{20}		207	71	i aq; misc alc, eth
d17	Decanoyl chloride	$CH_3(CH_2)_8C(=0)Cl$	190.71	2,356	0.919	1.4410^{20}	-34.5	96 ^{5mm}	98	d aq, alc; s eth
d18	1-Decene	$CH_3(CH_2)_7CH = CH_2$	140.27	1 ³ , 858	0.7408_4^{20}	1.4215^{20}	-66.3	170.6	47	i aq; misc alc, eth
d19	Decylamine	CH ₃ (CH ₂) ₉ NH ₂	157.30	4, 199	0.787	1.4360^{20}	12–14	216–218	85	sl s aq; misc alc, bz, eth, acet
d20	Dehydroabietylamine		285.48			1.5460^{20}			>112	
d21	Dehydroacetic acid		168.15	17, 559			111–113	269.9		22 acet; 18 bz; 5 MeOH
d22	Deoxybenzoin	$C_6H_5CH_2C(=O)C_6H_5$	196.25	7, 431	1.201_4^0		55-56	320		i aq; v s alc, eth

Cymenes, i100, i101, i102 4-Cymylphenol, m359 Cysteamine, a162 Cysteic acid hydrate, a288 Cytosine, a198 2,4-D, d214 p,p'-DDT, b167 1,2-Decahydroacenaphthylene, a2 Decamethylene glycol, d10 1,10-Decadedicarboxylic acid, d721 Decyl aldehyde, d6 Decyl chloride, c80 Decyl iodide, i33 Dextrose, g6

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d23	Diacetoxydimethyl-	(CH ₃) ₂ Si(OOCCH ₃) ₂	176.3		1.054 ²⁰	1.4030 ²⁰		164–166		
d24	silane Diacetoxymethyl- phenylsilane	$CH_3(C_6H_5)Si (OCOCH_3)_7$	238.3			1.487 ²⁰		127 ^{6mm}		
d25	Diallylamine	(H ₂ C=CHCH ₂) ₂ NH	97.16	4, 208	0.787	1.4405^{20}	-88	111-112	15	
d26	Diallyl ether	$(H_2C = CHCH_2)_2O$	98.15	$1^2,477$	0.805^{18}_{0}	1.4240^{20}		94		i aq; misc alc, eth
d27	Diallyl sulfide	$(H_2C = CHCH_2)_2S$	114.21	1,440	0.8877_4^{27}	1.4889^{20}	-83	138	46	sl s aq; misc alc,
				_						eth
d28	1,2-Diaminoanthra- quinone		238.25	14 ¹ , 459			289–291			sl s alc, eth
d29	1,4-Diaminoanthra- quinone		238.25	14, 197			265–268			sl s aq, alc; v s bz
d30	2,6-Diaminoanthra- quinone		238.25	14, 215			>325			sl s hot aq, pyr
d31	2,5-Diaminoazo- benzene HCl	$C_6H_5N=NC_6H_3-$ $(NH_2)_2\cdot HCl$	248.72	16, 383			235 d			
d32	2,5-Diaminobenzene- sulfonic acid	$(H_2N)_2C_6H_3SO_3H$	188.21	14,713			298 d			sl s aq, alc
d33	3,5-Diaminobenzoic	$(H_2N)_2C_6H_3COOH$	152.15	14, 453			228	-H ₂ O, 110		sl s aq; s alc, eth
d34	4,4'-Diaminodiphenyl-	H ₂ NC ₆ H ₄ NHC ₆ H ₄ - NH ₂ ·H ₂ SO ₄	297.33	13, 110			300			
d35	4,4'-Diaminodiphenyl- methane	H ₂ NC ₆ H ₄ CH ₂ C ₆ H ₄ NH ₂	198.27	13, 238			91–92	398	221	sl s aq; v s alc, bz,
d36	3,3'-Diaminodiphenyl sulfone	H ₂ NC ₆ H ₄ SO ₂ C ₆ H ₄ NH ₂	248.30	13, 426			167–170			i aq; s alc, bz
d37	4,4'-Diaminodiphenyl sulfone	H ₂ NC ₆ H ₄ SO ₂ C ₆ H ₄ NH ₂	248.30	13, 536			175–177			i aq; s alc, acet, HCl
d38	2,7-Diaminofluorene		196.25	13, 266			165–166			sl s aq; v s alc

d39	2,4-Diamino-6- hydroxypyrimidine		126.12	24, 469			285 d			s aq
d40	Diaminomaleonitrile	$NCC(NH_2) = C(NH_2)CN$	108.10	$4^2,949$			178–179			
d41	1,8-Diamino- <i>p</i> -menthane		170.30	13, 4	0.914	1.4805^{20}	-45	107- 125 ^{10mm}	93	
d42	3,3'-Diamino- <i>N</i> -	CH ₃ N[(CH ₂) ₃ NH ₂],	145.25	4 ⁴ , 1279				110-	102	
	methyl-	3 4 23 22						112 ^{6mm}		
	dipropyamine									

Diacetins, g17, g18 Diacetone acrylamide, d568 Diacetone alcohol, h142 Diacetonitrile, a151 (Diacetoxyiodo)benzene, i28 Diacetyl, b386 Diallyl, h41
2,5-Diaminoanisole, m94
1,4-Diaminobutane, b379
1,2-Diaminocyclohexanes, c318, c319
1,10-Diaminodecane, d8
p-Diaminodiphenyl, b136

3,3'-Diaminodipropylamine, i9 1,12-Diaminododecane, d720 1,2-Diaminoethane, e15 1,7-Diaminoheptane, h7 1,6-Diaminohexane, h56

NH₂

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d43	1,3-Diamino-2-	H ₂ NCH ₂ CH(OH)CH ₂ NH ₂	90.13	4, 290			40–45	235		
d44 d45	propanol 2,6-Diaminopyridine 1,4-Diazabicyclo- [2.2.2]octane	(H ₂ N) ₂ C ₅ H ₃ N	109.13 112.18	221,647			118–120 158	174		s aq, alc 45 aq; 77 EtOH; 51 bz; 13 acet; 26 MeEtKe
d46	1,8-Diazabicyclo- [5.4.0]undec-7-ene		152.24		1.018	1.5219 ²⁰		80 ^{0.6mm}	>112	20 WELLIKE
d47	Diazomethane	CH ₂ =N=N	42.04	23, 25			-145	-23	very exp- losive	s eth, diox
d48	1-Diazo-2-naphthol- 4-sulfonic acid, Na salt		272.22	16, 595			166		103110	
d49	Dibenz[de,kl]anthra- cene		252.32	51, 363	1.35		273–274	503		s bz; sl s alc, eth
d50	Dibenzofuran		168.20	17, 70	1.0886499	1.607999	81–83	285		i aq; s alc, bz, eth
d51	2,3,11,12-Dibenzo- 1,4,7,10,13-hexa- oxacyclooctadeca- 2,11-diene		360.41				162–164			
d52	Dibenzothiophene		184.26	17,72			97.100	332–333		s aq; v s alc, bz
d53	Dibenzoylmethane	$C_6H_5C(=O)CH_2-$ $C(=O)C_6H_5$	224.26	7,769			78–79	220 ^{18mm}		s alc; v s eth
d54	Dibenzoly peroxide	C ₆ H ₅ C(O)O— OC(O)C ₆ H ₅	242.23				103–106	may explode when heated		sl s aq, alc; s bz, chl, eth

d55	(—)-Dibenzoyl-L- tartaric acid	$[(C_6H_5COOCH-(COOH)]_2 \cdot H_2O$	376.34	9, 170						
d56	hydrate Dibenzylamine	C ₆ H ₅ CH ₂ NHCH ₂ C ₆ H ₅	197.28	12, 1035	1.026	1.5731 ²⁰	-26	300	143	i aq; s alc, eth
d57	Dibenzyl disulfide	C ₆ H ₅ CH ₂ SSCH ₂ C ₆ H ₅	246.39	6, 465			69	d > 270		s hot alc, bz, eth
d58	Dibenzyl ether	C ₆ H ₅ CH ₂ OCH ₂ C ₆ H ₅	198.27	6, 434	1.0014_4^{20}	1.5610^{20}	3.5	298 d	135	misc alc, acet, chl,
										eth

1,3-Diamino-2-hydroxypropane, d43

Diaminonaphthalenes, n4, n5

1,2-Diamino-4-nitrobenzene, n68

1,4-Diamino-2-nitrobenzene, n67

1,9-Diaminononane, n93

1,8-Diaminooctane, o23

1,5-Diaminopentane, p29

2,5-Diaminopentanoic acid, o46

1,2-Diaminopropane, p192

1,3-Diaminopropane, p193

4,6-Diamino-4-pyrimidinol, d39

Diaminotoluenes, t168, t169, t170, t171

1,3-Diaminourea, c11

4,5-Diamino-o-xylene, d586

Diamylamine, d650

Diamyl ether, d651

Diamyl ketone, u6

1,2-Dianilinoethane, d669

Diazoacetic ester, e114 1.3-Diazole, i4 Dibenzo-18-crown-6, d51 Dibenzo[b,e]pyridine, a61 Dibenzopyrrole, d665 Dibenzoyl, b34 Dibenzyl, d666

d46

d51

d49

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d59	N,N'-Dibenzylethyl- enediamine	(C ₆ H ₅ CH ₂ NHCH ₂ —) ₂	240.35	12, 1067	1.024 ²⁰	1.5624 ²⁰	26	195 ^{4mm}	>112	v s alc, bz, chl, eth
d60 d61 d62	Dibenzyl malonate Dibenzyl phosphonate Dibromoacetic acid	CH ₂ [COOCH ₂ C ₆ H ₅] ₂ (C ₆ H ₅ CH ₂ O) ₂ P(O)H Br ₂ CHCOOH	284.31 262.25 217.86	6, 436	1.137 1.187	$1.5447^{20} 1.5540^{20}$	-5 to +5	188 ^{0.2mm} 110 ^{0.01mm} 128–	>112 >112	
d63	Dibromoacetonitrile	Br ₂ CHCN	198.86	2, 219	2.296	1.5393 ²⁰		130 ^{16mm} 67– 69 ^{24mm}	none	
d64	2,4'-Dibromoaceto- phenone	$BrC_6H_4C(=O)CH_2Br$	277.96	7, 285			108–110	0)		s warm alc, eth
d65	1,4-Dibromobenzene	$C_6H_4Br_2$	235.92	5, 211	0.9641100	1.5743100	87.3	219	none	1.4 alc; s bz; 101 eth
d66	4,4'-Dibromobiphenyl	BrC ₆ H ₄ C ₆ H ₄ Br	312.00	5,580			162-163	355-360		s bz; sl s hot alc
d67	1,3-Dibromobutane	CH ₃ CH(Br)CH ₂ CH ₂ Br	215.93	1, 120	1.800^{20}	1.5085^{20}		175	none	s chl, eth
d68	1,4-Dibromobutane	BrCH ₂ CH ₂ CH ₂ CH ₂ Br	215.93	1, 120	1.8080^{20}_{4}	1.5186^{20}	-20	198	>112	s chl
d69	1,4-Dibromo-2,3- butanedione	$BrCH_2C(=O)C(=O)$ -	243.89	1,774	-		116–117			
d70	trans-2,3-Dibromo-2- butene-1,4-diol	$HOCH_2C(Br) = C(Br)$	245.91	11, 260			112–114			
d71	Dibromo- chloromethane	HCClBr ₂	208.29	1, 67	2.451	1.5465 ²⁰	-22	120 ^{748mm}	none	misc alc, bz, eth
d72	1,2-Dibromo-2- chloro-1,1,2-tri- fluoroethane	FCCl(Br)C(Br)F ₂	276.5		2.2478 ²⁰	1.4275 ²⁰		93–94		
d73	1.10-Dibromodecane	Br(CH ₂) ₁₀ Br	300.09	1 ¹ , 64	1.33530	1.4912^{20}	27	160 ^{15mm}	>112	sl s alc; s eth
d74	,	2710		1 '	2.223820	1.4456^{20}		93.4		i aq
	difluoroethane			, ,						1
d75	Dibromodifluoro- methane	Br ₂ CF ₂	209.81	11, 16	2.28845	1.399912	-141.6	23–24	none	0.1 aq; misc alc, bz, chl, eth
d67 d68 d69 d70 d71 d72	1,3-Dibromobutane 1,4-Dibromobutane 1,4-Dibromo-2,3- butanedione trans-2,3-Dibromo-2- butene-1,4-diol Dibromo- chloromethane 1,2-Dibromo-2- chloro-1,1,2-tri- fluoroethane 1,10-Dibromodecane 1,2-Dibromo-1,1- difluoroethane Dibromodifluoro-	CH ₃ CH(Br)CH ₂ CH ₂ Br BrCH ₂ CH ₂ CH ₂ CH ₂ Br BrCH ₂ C(=O)C(=O)- CH ₂ Br HOCH ₂ C(Br)=C(Br)- CH ₂ OH HCClBr ₂ FCCl(Br)C(Br)F ₂	215.93 215.93 243.89 245.91 208.29 276.5	1, 120 1, 120 1, 774 1, 774 1, 260 1, 67	$ \begin{array}{c} 1.8080_{4}^{20} \\ 2.451 \\ 2.2478^{20} \\ 1.335^{30} \\ 2.2238^{20} \end{array} $	1.5186 ²⁰ 1.5465 ²⁰ 1.4275 ²⁰ 1.4912 ²⁰ 1.4456 ²⁰	-20 116-117 112-114 -22 27 -61.3	175 198 120 ⁷⁴⁸ⁿ 93–94 160 ^{15m} 93.4	mm m	none >112 none >112

d76	1,3-Dibromo-5,5-di- methylhydantoin		285.93				197 d			
d77	1,1-Dibromoethane	CH ₃ CHBr ₂	187.87	1,90	2.055_4^{20}	1.5379^{20}		113		i aq; v s alc, eth
d78	1,2-Dibromoethane	BrCH ₂ CH ₂ Br	187.87	1,90	2.1802_4^{20}	1.5416 ¹⁵	10.0	131.7	none	0.43 aq; misc alc,
d79	(1,2-Dibromoethyl)- benzene	C ₆ H ₅ CH(Br)CH ₂ Br	263.97	5, 356			70–74	140 ^{15mm}		eth
d80	cis-1,2-Dibromo-	BrCH=CHBr	185.86	1, 190	2.21_4^{17}	1.543118	-53	112.5		s alc, bz, chl, eth
	ethylene									
d81	trans-1,2-Dibromo- ethylene	BrCH=CHBr	185.86	1, 190	2.246	1.550518	-6.5	108		
d82	1,2-Dibromoethyltri-	BrCH ₂ CH(Br)SiCl ₃	321.3		2.046_4^{20}	1.53720		90 ^{11mm}		
402	chlorosilane	Breri ₂ err(Br)Srei ₃	321.3		2.0404	1.557		70		
d83	4',5',-Dibromofluo-		490.12	19, 228			270-273			s hot alc, HOAc
	rescein									
d84	2,4-Dibromo-1-fluoro- benzene	$Br_2C_6H_3F$	253.91		2.047 ²⁰	1.5840 ²⁰		105 ^{22mm}	92	
d85	1,2-Dibromohexa-	$CF_3CF(Br)C(Br)F_2$	309.83				72.8			
	fluoropropane									

Dibenzyl ketone, d684

5,7-Dibromo-8-quinolinol, d87

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d86 d87	1,6-Dibromohexane 5,7-Dibromo-8- hydroxyquinoline	Br(CH ₂) ₆ Br	243.98 302.96	1, 145 21, 97	1.58648	1.5066 ²⁰	200–201	243 subl	32	misc eth s alc, bz; v s eth
d88	Dibromomethane	CH_2Br_2	173.85	1,67	2.4956_4^{20}	1.5419 ²⁰	-52.7	96.97	none	1.15 aq; misc alc, bz, acet, chl, eth
d89	2,6-Dibromo-4-nitro- aniline	$Br_2C_6H_2(NO_2)NH_2$	295.93	12, 743			206–208			sl s aq; s HOAc
d90	2,5-Dibromonitro- benzene	$Br_2C_6H_3NO_2$	280.91	5, 250	1.9581111		82–84			s bz, hot alc
d91	1,5-Dibromopentane	Br(CH ₂) ₅ Br	229.95	1, 131	1.6879_4^{15}	1.5092^{15}	-34	110 ^{15mm}	79	
d92	1,2-Dibromopropane	CH ₃ CH(Br)CH ₂ Br	201.90	1, 109	1.93320	1.5203^{20}	-55.5	139.6	none	0.2 aq; misc alc, bz, chl, eth
d93	1,3-Dibromopropane	BrCH ₂ CH ₂ CH ₂ Br	201.90	1, 110	1.9712_4^{25}	1.5233^{20}	-34	166.8	54	0.17 aq; s alc, eth
d94	2,3-Dibromopropanol	BrCH ₂ CH(Br)CH ₂ OH	217.90	1, 357	2.120_4^{20}	1.5599 ²⁰		95–97 ^{10mm}		sl s aq; misc alc, bz, eth, acet
d95	2,3-Dibromopropene	$BrCH_2C(Br) = CH_2$	199.88	1, 201	1.9336_4^{20}	1.5470^{20}		140-143	none	
d96	2,3-Dibromopropionic acid	BrCH ₂ CH(Br)COOH	231.88	2, 258			64–66	160 ^{20mm}		s aq, alc, bz
d97	2,6-Dibromopyridine	$Br_2(C_5H_3N)$	236.91	20^2 , 153			118-119	255		
d98	DL-2,3-Dibromo- succinic acid	HOOCCH(Br)CH(Br)- COOH	275.89	2, 625			167			v s aq, alc
d99	1,2-Dibromotetra- chloroethane	BrCCl ₂ CCl ₂ Br	325.65	1,93	2.713		220–222		none	
d100	1,2-Dibromotetra- fluoroethane	BrCF ₂ CF ₂ Br	259.83		2.16325	1.367 ²⁵	-110.5	47.3		
d101	2,5-Dibromothiophene	$Br_2C_4H_2S$	241.94	17, 33	2.147_{23}^{23}	1.6289^{20}	-6	221		i aq; v s alc, eth
d102	α, α -Dibromotoluene	C ₆ H ₅ CHBr ₂	249.94	5, 308	1.51015	1.6147^{20}		156 ^{23mm}	110	i aq; misc alc, eth
d103	1,2-Dibromo-1,1,2-	HC(Br)FC(Br)F ₂	241.8	1,92	$2,274^{27}$	1.4191^{24}		76.5		
	trifluoroethane	· · · · -								

d104	α, α' Dibromo- o -	$C_6H_4(CH_2Br)_2$	263.97	5, 366	1.960		92–94			sl s alc, chl, eth
d105	xylene α, α' -Dibromo- p - xylene	$C_6H_4(CH_2Br)_2$	263.97	5, 385	2.0120		142–143	245		v s alc, chl; s eth
d106	1,2-Dibutoxyethane	C ₄ H ₉ OCH ₂ CH ₂ OC ₄ H ₉	174.28		0.8374_{20}^{20}	1.4131^{20}	-69.1	203.6		0.2 aq; misc alc, acet
d107	Dibutylamine	$(C_4H_9)_2NH$	129.25	4, 157	0.7601_4^{20}	1.4177^{20}	-62	159.6	33	0.47 aq; s alc, acet, eth, EtAc, PE
d108	N,N-Dibutylamino- ethanol	(C ₄ H ₉) ₂ NCH ₂ CH ₂ OH	173.29		0.860_{20}^{20}	1.444^{20}	<-70	227–230	93	eu., 2u.10, 1 2
d109	N,N-Dibutylaniline	$C_6H_5N(C_4H_9)_2$	205.34	12 ² , 95	0.90420	1.5197 ²⁰		267–275	110	i aq, MeOH; s acet, bz, EtOH, EtAc, eth
d110	Dibutyl decanedioate	C ₄ H ₉ OOC(CH ₂) ₈ COO- C ₄ H ₉	314.45	2,719	0.9366 ²⁰	1.4415^{20}	1.0	344–345	177	0.004 aq
d111	Di- <i>tert</i> -butyldi- carbonate	(CH ₃) ₃ COC(O)OC- (CH ₃) ₃	218.25		0.950	1.4103^{20}	23	56 ^{0.5mm}	37	
d112	2,5-Di- <i>tert</i> -butyl- 1,4-dihydroxy- benzene	[(CH ₃) ₃ C] ₂ C ₆ H ₂ (OH) ₂	222.33				217–219			
d113	Dibutyl disulfide	$C_4H_9SSC_4H_9$	178.36	$1^2,400$	0.9383_4^{20}	1.4920^{20}	-71	231.2	93	i aq; misc alc, eth

Dibutyl 1,2-benzenedicarboxylate, d128

Dibutyl butanedioate, d130

Dibutyl Cellosolve, d106

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d114	Di-tert-butyl disulfide	(CH ₃) ₃ CSSC(CH ₃) ₃	178.36		0.935	1.4920		229–33	93	
d115	Dibutyl ether	$C_4H_9OC_4H_9$	130.22	1, 369	0.7689_4^{20}	1.3992^{20}	-97.9	142.4	25	0.03 aq; misc alc,
d116	N,N-Dibutyl- formamide	$HC(=O)N(C_4H_9)_2$	157.26		0.864	1.4429^{20}		120 ^{15mm}	100	
d117	3,5-Di- <i>tert</i> -butyl-4-hy-droxybenzoic acid	[(CH ₃) ₃ C] ₂ C ₆ H ₂ - (OH)COOH	250.34				206–209			
d118	Dibutyl maleate	C ₄ H ₉ OOCCH= CHCOOC ₄ H ₉	228.28		0.9950^{20}	1.4454 ²⁰	<-80	d 280	135	0.05 aq
d119	Di-tert-butyl malonate	CH ₂ COOC(CH ₃) ₃	216.27			1.4184 ²⁰	-6.0	93 ^{10mm}		
		COOC(CH ₃) ₃								
d120	2,6-Di- <i>tert</i> -butyl-4- methylphenol	$[(CH_3)_3C]_2C_6H_2(CH_3)OH$	220.36	$6^3, 2073$	0.894_4^{75}	1.4859 ⁷⁵	70	265		i aq; s alc, bz, acet
d121	Dibutyl oxalate	C ₄ H ₉ OOC—COOC ₄ H ₉	202.25	2, 540	0.986_{20}^{20}	1.423220	-30.0	239–240	108	misc alc, ketones, PE
d122	Di- <i>tert</i> -butyl peroxide	$(CH_3)_3CO - OC(CH_3)_3$	146.23		0.794^{20}	1.3890^{20}	-40	110		misc acet, octane
d123	2,4-Di- <i>tert</i> -butyl-	[(CH ₃) ₃ C] ₂ C ₆ H ₃ OH	206.33				56.5	263.5	115	s hot alc; i alk
d124	2,6-Di- <i>sec</i> -butyl-	[CH ₃ CH ₂ CH(CH ₃)] ₂ - C ₆ H ₃ OH	206.33		0.918	1.5100^{20}	-42	255–260	127	
d125	2,6-Di- <i>tert</i> -butyl-phenol	[(CH ₃) ₃ C] ₂ C ₆ H ₃ OH	206.33	6^3 , 2061			35–83	253	118	s hot alc; i alk
d126	3,5-Di- <i>tert</i> -butyl-phenol	[(CH ₃) ₃ C] ₂ C ₆ H ₃ OH	206.33				87–89			
d127	Dibutyl phosphonate	$(C_4H_9O)_2P(O)H$	194.21	1, 187	0.995_4^{20}	1.4231 ²⁰		118 ^{11mm}	121	sl s (hyd) aq; misc alc, acet, eth
d128	Dibutyl o-phthalate	$C_6H_4[COOC_4H_9]_2$	278.35	9 ² , 586	1.04654	1.4926 ²⁰	-35	340	171	0.01 aq; v s alc, bz, acet, eth

d129	N,N-Dibutyl-1,3-	C ₄ H ₉ NHCH ₂ CH ₂ CH ₂ -	186.34		0.827	1.4463^{20}		205	103	I
u12)	propanediamine	NHC ₄ H ₉	100.51		0.027	1.1105		203	103	
d130	Dibutyl succinate	$[C_4H_9OOCCH_2-]_2$	230.30	2^2 , 551	0.9768_4^{20}	1.4299^{20}	-29.0	274.5		i aq; s alc, eth
d131	Dibutyl sulfate	C ₄ H ₉ OSO ₂ OC ₄ H ₉	210.29		1.059_4^{25}	1.4213^{20}		130-		
								132 ^{11mm}		
d132	Dibutyl sulfide	$C_4H_9SC_4H_9$	146.30	1,370	0.839_0^{16}	1.4530^{20}	-75.0	188.9	76	i aq; v s alc, eth
d133	Di- <i>tert</i> -butyl sulfide	$(CH_3)_3CSC(CH_3)_3$	146.30		0.815	1.4506^{20}		151	48	
d134	Dibutyl sulfite	$(C_4H_9O)_2S(O)$	194.29	1^2 , 397	0.9944_4^{22}	1.4310^{20}		108 ^{15mm}		
d135	Dibutyl sulfone	$(C_4H_9)_2SO_2$	178.29	1,371			46	295	143	i aq; s alc, eth
d136	N,N'-Dibutylthio-	$C_4H_9NHC(=S)NHC_4H_9$	188.34				63.65			i aq; s alc; sl s eth
	urea							40		
d136a	Dibutyltin dichloride	$(C_4H_9)_2SnCl_2$	303.83				39–41	135 ^{10mm}	>112	
d137	Dibutyltin oxide	$(C_4H_9)_2SnO$	248.92	4 ¹ , 588			>300			
d138	Dichloroacetic acid	Cl₂CHCOOH	128.94	2, 202	1.563 ₄ ²⁰	1.4642^{20}	9–11	193–194	>112	misc aq, alc, eth
d139	1,1-Dichloroacetone	CH ₃ C(O)CHCl ₂	126.97	1,654	1.30518			150		sl s aq; s alc; misc eth
d140	2',4'-Dichloroaceto- phenone	Cl ₂ C ₆ H ₃ COCH ₃	189.04	7 ² , 219		1.5635^{20}	33–34	145 ^{15mm}	>112	i aq
d141	Dichloroacetyl chloride	Cl ₂ CHCOCl	147.39	2, 204	1.5315 ₄ ¹⁶	1.4603 ²⁰		107–108	66	d aq, alc; misc eth
d142	2,3-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	12, 621		1.5969^{20}	23-24	252	>112	s alc; v s eth
d143	2,4-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	12, 621	1.56720		59.62	245		sl s aq; s alc, eth
d144	2,5-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 625			49–51	251		s alc, bz, eth

Di-*tert*-butylcresol, d120 2,5-Di-*tert*-butylhydroquinone, d112 Dibutyl ketone, n100 Dibutyl phosphite, d127 Dibutyl sebacate, d110

Dichloroacetaldehyde diethyl acetal, d169

Dichloroanisoles, d191, d192

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d145	2,6-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	12, 626			38.41			
d146	3,4-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	12,626			70–72	272		s alc, eth; sl s bz
d147	3,5-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	12,626			51-53	259 ^{741mm}		i aq; s alc, eth
d148	1,5-Dichloroanthra-		277.11	7,787			245-247			sl s alc, bz, acet
	quinone									
d149	1,8-Dichloroanthra-		277.11	7,788			202-203			sl s alc
	quinone									
d150	2,4-Dichlorobenz-	Cl ₂ C ₆ H ₃ CHO	175.01	7, 236			69-73	233		i aq; s alc
	aldehyde									1
d151	2,4-Dichlorobenz-	Cl ₂ C ₆ H ₃ CONH ₂	190.03	9 ³ , 1376			191-194			
	amide									
d152	1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.01	5, 201	1.3059_4^{20}	1.5515	-17.0	180.4	65	misc alc, bz, eth
d153	1,3-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.01	5, 202	1.2884_4^{20}	1.5459	-24.8	173.1	63	0.01 aq; s alc, eth
d154	1,4-Dichlorobenzene	$C_6H_4Cl_2$	147.01	5, 203	1.241760	1.5285	53	174.1	65	s alc, bz, chl, eth
d155	2,5-Dichlorobenzene-	Cl ₂ C ₆ H ₃ SO ₂ Cl	245.51	11 ¹ , 15			36–37			d hot aq, hot alc
	sulfonyl chloride									
d156	2,4-Dichlorobenzoic	Cl ₂ C ₆ H ₃ COOH	191.01	9, 342			157-160			s hot aq, alc, bz,
	acid									chl
d157	2,5-Dichlorobenzoic	Cl ₂ C ₆ H ₃ COOH	191.01	9, 342			151-154	301		sl s aq; s alc,
	acid									eth
d158	3,4-Dichlorobenzoic	Cl ₂ C ₆ H ₃ COOH	191.01	9, 343			207-209			s hot aq, eth; v s
	acid									alc
d159	4,4'-Dichlorobenzo-	(ClC ₆ H ₄) ₂ CO	251.11	7,420			144–146	353		s hot alc; v s chl,
	phenone									eth
d160	2,4-Dichlorobenzoyl	Cl ₂ C ₆ H ₃ COCl	209.46	9, 342	1.494	1.5297^{20}	16-18	150 ^{34mm}	137	d aq, alc
	chloride									
d161	3,4-Dichlorobenzoyl	Cl ₂ D ₆ H ₃ COCl	209.46	9, 344			30–33	242	142	d aq, alc
	chloride									
d162	1,2-Dichlorobutane	CH ₃ CH ₂ CH(Cl)CH ₂ Cl	127.01	11,38	1.118_4^{20}	1.4474 ¹⁵		124		i aq; s chl, eth
	I	I		I	ı	I	ı	I	1	I

d163	1,4-Dichlorobutane	CICH ₂ CH ₂ CH ₂ CH ₂ CI	127.01	1, 119	1.1598_4^{20}	1.4566^{20}	-38	155	40	i aq; s chl
d164	<i>meso</i> -2,3-Dichloro-butane	CH ₃ CH(Cl)CH(Cl)CH ₃	127.01	1, 119	1.1025_4^{25}	1.4386 ²⁵	-80	115.9	18	i aq; s chl
d165	cis-1,4-Dichloro- 2-butene	CICH ₂ CH=CHCH ₂ Cl	125.00	$1^3,743$	1.188_4^{25}	1.4887 ²⁵	-48	152	49	i aq; s org solv
d166	trans-1,4-Dichloro- 2-butene	CICH ₂ CH=CHCH ₂ Cl	125.00	$1^3,743$	1.183425	1.4861 ²⁵	1–3	74–76 ^{40mm}	56	i aq; s org solv
d167	3,4-Dichloro-1- butene	CICH ₂ CH(Cl)CH=CH ₂	125.00		1.150	1.4658 ²⁰	-61	123	28	
d168	1,4-Dichloro-2- butyne	ClCH ₂ C≡CCH ₂ Cl	122.98	$1^3,927$	1.258420	1.5048^{20}		165–168	160	
d169	1,1-Dichloro-2,2-di- ethoxyethane	Cl ₂ CHCH(OC ₂ H ₅) ₂	187.07	1,614	1.138	1.4360^{20}		183–184	60	
d170	Dichlorodifluoro- methane	Cl ₂ CF ₂	120.92	1,61	1.486^{-30}		-158	-29.8		0.02 aq; 9 bz; 5.5 chl; 6 diox; s alc, eth
d171	4,6-Dichloro-1,3-di- hydroxybenzene	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179.00	61, 403			104–106	254		sl s aq, bz; s eth
d172	2,5-Dichloro-3,6-di- hydroxy- <i>p</i> -benzo-		208.98	8, 379			283–284			
	quinone		I		I		I	I		I

2,6-Dichlorobenzyl chloride, t249 2,2'-Dichlorodiethyl ether, b158

5,5'-Dichloro-2,2'-dihydroxydiphenylmethane, m233

1,1-Dichlorodimethyl ether, d197 Dichlorohydrin, d220

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d173	1,3-Dichloro-3,5-di-		197.02	24 ² , 158			134–136			
d174	methylhydantoin Dichlorodimethyl- silane	(CH ₃) ₂ SiCl ₂	129.06		1.06420	1.4038 ²⁰	-16	70	-16	
d175	Dichlorodiphenyl- silane	$(C_6H_5)_2SiCl_2$	253.20	16,910	1.222_4^{20}	1.58220		308–309	157	d aq, alc
d176 d177	1,1-Dichloroethane 1,2-Dichloroethane	CH ₃ CHCl ₂ CICH ₂ CH ₂ Cl	98.96 98.96	1, 83 1, 84	$ \begin{array}{c c} 1.1757_4^{20} \\ 1.2531_4^{20} \end{array} $	$ \begin{array}{c} 1.4164^{20} \\ 1.4448^{20} \end{array} $	-97.0 -35.7	57.3 83.5	-5 15	0.51 aq; misc alc 0.8 aq; misc alc, chl, eth
d178	1,1-Dichloroethylene	H ₂ C=CCl ₂	96.94	1, 186	1.2129_4^{20}	1.4247 ²⁰	-122.6	31.6	-15	0.02 aq; s alc, bz, chl, eth
d179	cis-1,2-Dichloro- ethylene	CICH=CHCl	96.94	1, 188	1.2818420	1.4490^{20}	-80.1	60.7	6	0.7 aq; s alc, eth
d180	trans-1,2-Dichloro- ethylene	CICH=CHCl	96.94	1, 188	1.2546420	1.446220	-49.8	47.7	6	0.6 aq; s alc, eth
d181	2,2'-Dichloroethyl	CICH ₂ CH ₂ OCH ₂ CH ₂ Cl	143.01	1 ² , 335	1.2220_{20}^{20}	1.457 ²⁰		178.5	55	1.1 aq; s alc, bz,
d182	1,2-Dichloroethyl- trichlorosilane	ClCH ₂ CH(Cl)SiCl ₃	232.4		1.516 ₄ ²⁵	1.449 ²⁵		82- 84 ^{26mm}		
d183	Dichlorofluoro- methane	FCHCl ₂	102.92	1,61	1.345 ³⁰		-135	8.9		69 HOAc; 108 diox; s alc, eth; i aq
d184	Dichloroheptyl- methylsilane	C ₇ H ₁₅ Si(CH ₃)Cl ₂	225.2		0.9780_4^{20}	1.4396 ²⁵		207–208		1 44
d185	1,2-Dichlorohexa- fluorocyclobutane	F ₆ C ₄ Cl ₂	233.0			1.3342 ²⁵		59–60		
d186	1,5-Dichlorohexa- methyltrisiloxane	[ClC(CH ₃) ₂ O] ₂ - Si ₃ (CH ₃) ₂	277.4		1.018_4^{20}	1.4071		184		
d187	1,6-Dichlorohexane	Cl(CH ₂) ₆ Cl	155.07	1, 144	1.068	1.4568^{20}		87 ^{15mm}	73	s chl

d188	1,2-Dichloro-2-iodo- 1,1,2-trifluoro- ethane	F(I)C(Cl)C(Cl)F ₂	278.9		2.200 ²⁰	1.4490 ²⁰		100–101		
d189	Dichloromaleic anhydride		166.95	17, 434						
d190	Dichloromethane	CH ₂ Cl ₂	84.93	1,60	1.3255 ²⁰	1.4246 ²⁰	-96.7	40.5	none	1.3 aq; misc alc, eth
d191	2,3-Dichloro-1- methoxybenzene	Cl ₂ C ₆ H ₃ OCH ₃	177.03	6 ¹ , 102			31–33			
d192	3,5-Dichloro-1- methoxybenzene	Cl ₂ C ₆ H ₃ OCH ₃	177.03	6, 190			40–42			
d193	2,4-Dichloro-6-meth- oxy-1,3,5-triazine		179.99				86–88	132 ^{49mm}		
d194	(Dichloromethyl)di- methylchlorosilane	Cl ₂ CHSi(Cl)(CH ₃) ₂	177.5		1.237420	1.461 ²⁰	-49	149		
d195	2,2-Dichloro-1- methylcyclo- propane-	Cl ₂ (C ₃ H ₂)(CH ₃)COOH	169.01				60–65	85 ^{8mm}		
1106	carboxylic acid	G H N GGI	171.02	10 447	1.265	1 571020		10 < 30mm	70	
d196	N-(Dichloromethylene)aniline	$C_6H_5N=CCl_2$	174.03	12, 447	1.265	1.5710^{20}		106 ^{30mm}	79	
d197	Dichloromethyl ether	Cl ₂ CHOCH ₃	114.96		1.271	1.4300^{20}		85	42	

Dichloroisopropyl alcohol, d220

4,4'-Dichloro-α-methylbenzhydrol, b164

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d198	Dichloro(methyl)- phenylsilane	C ₆ H ₅ Si(CH ₃)Cl ₂	191.13		1.176	1.519020		205	82	
d199	Dichloro(methyl)- silane	HSi(CH ₃)Cl ₂	115.04	4 ¹ , 581	1.105		-93	41	-32	
d200	Dichloro(methyl)- vinylsilane	H ₂ C=CHSi(CH ₃)Cl ₂	141.07		1.087 ₄ ²⁰	1.4300^{20}		92–93	4	
d201	2,3-Dichloro-1,4- naphthoquinone		227.05	7,729			190–192			sl s alc, bz, eth
d202	2,6-Dichloro-4- nitroaniline	Cl ₂ C ₆ H ₂ (NO ₂)NH ₂	207.02	12, 735			190–192			
d203	2,3-Dichloronitro- benzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	5, 245	1.72114		61–62	257–258		s PE
d204	2,4-Dichloronitro- benzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	5, 245	1.43980		29–32	258		s hot alc; misc eth
d205	3,4-Dichloronitro- benzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	5, 246	1.456 ⁷⁵		41–42	255–256	123	
d206	2,3-Dichloroocta- fluorobutane	CF ₃ CF(Cl)CF(Cl)CF ₃	271.0		1.6801 ²⁰	1.3100^{20}	-68	63		
d207	1,7-Dichloroocta- methyltetrasiloxane	[Cl(CH ₃) ₂ SiOSi- (CH ₃) ₂ —] ₂ O	351.6		1.011_4^{20}	1.403^{20}		222		
d208	2,3-Dichloro-4-oxo- 2-butenoic acid	ClC(CHO)=C(Cl)COOH	168.96	3,727			125–128		100	sl s aq; s alc, hot bz
d209	1,5-Dichloropentane	Cl(CH ₂) ₅ Cl	141.04	1, 131	1.105845	1.4553^{20}	-72	63 ^{10mm}	26	i aq; s alc, eth
d210	2,3-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	6 ¹ , 102			58.60	206		s alc, eth
d211	2,4-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	6, 189			42-43	210	113	v s alc, bz, chl, eth
d212	2,5-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	6, 189			56–58	211		v s alc, bz, eth
d213	2,6-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	6, 190			65–68	218-220		v s alc, eth
d214	2,4-Dichlorophenoxy-	Cl ₂ C ₆ H ₃ OCH ₂ COOH	221.04				138	160 ^{0.4mm}		s alc, bz, chl, eth
	acetic acid									

d215	2,5-Dichloro-p-	$Cl_2C_6H_2(NH_2)_2$	177.03	13, 118		ĺ	165 d	1		l
	phenylenediamine	2 0 21 22								
d216	Dichlorophenyl-	C ₆ H ₅ PCl ₂	178.99	16, 763	1.319	1.5980^{20}	-51	222	>112	
	phosphine									
d217	4,5-Dichloro-o-	$Cl_2C_6H_2(COOH)_2$	235.02	9 ¹ , 366			193-195			s aq; v s eth
	phthalic acid									
d218	1,2-Dichloropropane	CH ₃ CH(Cl)CH ₂ Cl	112.99	1, 105	1.155820	1.4390^{20}	-100.4	96.4	4	0.26 aq; misc alc,
										bz, chl, eth
d219	1,3-Dichlopropane	ClCH ₂ CH ₂ CH ₂ Cl	112.99	1, 105	1.878_4^{20}	1.4487^{20}	-99.5	120.5	32	v s alc, eth
d220	1,3-Dichloro-2- propanol	ClCH ₂ CH(OH)CH ₂ Cl	128.99	1,364	1.3506_4^{17}	1.4835^{20}	-4	174.3	74	9.1 aq; misc alc, eth
d221	* *	CICH,CH=CHCl	110.97	1, 199	1.217_4^{20}	1.470^{20}		112		
	1,3-Dichloropropene	_							10	i aq; s chl, eth
d222	2,3-Dichloro-1- propene	$ClCH_2C(Cl) = CH_2$	110.97	1, 199	1.204_{25}^{25}	1.4611^{20}		94	10	misc alc; s eth
d223	3,6-Dichloropyri-		148.98				66-69			
	dazine									
d224	2,6-Dichloropyridine	$Cl_2(C_5H_3N)$	147.99	20, 231			86-88			
d225	4,7-Dichloro-		198.05				84-86	148 ^{10mm}		
	quinoline									
d226	Dichlorosilane	H ₂ SiCl ₂	101.0				-122	8.3		
d227	1,2-Dichloro-	CICF ₂ CF ₂ CI	170.93		1.470_4^{20}	1.290^{20}	-94	3.6		s alc, eth
	1,1,2,2-tetrafluoro-									
	ethane									

1,1-Dichloro-2-propanone, d139

4,6-Dichlororesorcinol, d171

 α ,o-Dichlorotoluene, c59

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d228	2,5-Dichlorothio- phene	Cl ₂ (C ₄ H ₂ S)	153.03	17, 33	1.442	1.562120	-40.5	162		i aq; misc alc, eth
d229 d230 d231 d232	2,4-Dichlorotoluene 2,6-Dichlorotoluene 3,4-Dichlorotoluene 2,2-Dichloro-1,1,1- trifluoroethane	Cl ₂ C ₆ H ₃ CH ₃ Cl ₂ C ₆ H ₃ CH ₃ Cl ₂ C ₆ H ₃ CH ₃ CF ₅ CHCl ₂	161.03 161.03 161.03 152.9	5, 295 5, 296 5, 296	$ \begin{array}{c} 1.2460_{20}^{20} \\ 1.254 \\ 1.251_{25}^{25} \end{array} $	1.5454 ²⁰ 1.5507 ²⁰ 1.5472 ²⁰	-13 -14	200.5 196–203 201 ^{740mm} 28	79 82 85	i aq i aq; s chl i aq
d233	α, α' -Dichloro- p - xylene	C ₆ H ₄ (CH ₂ Cl) ₂	175.06	5, 384			100	254		22.5 acet; 20 bz; 4.5 CCl ₄ ; 11 eth; 18 EtAc
d234	2,5-Dichloro- <i>p</i> -xylene	$Cl_2C_6H_2(CH_3)_2$	175.06	5, 384			71	222		27 acet; 44 bz; 39 eth 32 EtAc; 5 MeOH
d235 d236	Dicyanodiamide 1,2-Dicyanobenzene	H ₂ NC(=NH)NHCN C ₆ H ₄ (CN) ₂	84.08 128.13	3 ² , 75 9, 815	1.400425		208–211 139–141			2.3 aq; 1.3 alc; i bz v s bz, alc; s hot eth
d237 d238 d239 d240	1,3-Dicyanobenzene 1,4-Dicyanobutane 1,6-Dicyanohexane 2,4-Dicyano-3- methylglutaramide	C ₆ H ₄ (CN) ₂ NC(CH ₂) ₄ CN NC(CH ₂) ₆ CN CH ₃ CH[CH(CN)- CONH ₃],	128.13 108.14 136.20 194.19	9, 836 2, 653 2, 694 2 ² , 704	0.951 0.954	1.4380 ²⁰ 1.4436 ²⁰	158–160 1–3 –3.5 159–160	295 185 ^{15mm}	>112 >112	s alc, bz, chl, eth
d241	Dicyclohexyl	$C_6H_{11}C_6H_{11}$	166.31	5, 108	0.864	1.4782 ²⁰	3–4	227	101	7 MeOH; misc bz, acet, eth
d242	Dicyclohexylamine	$(C_6H_{11})_2NH$	181.32	12, 6	0.910	1.484220	-0.1	255.8	96	misc alc, bz, chl,
d243	N, N' -Dicyclohexyl- carbodiimide	$C_6H_{11}N=C=NC_6H_{11}$	206.33				34–35	122- 124 ^{6mm}		
d244	Dicyclopentadiene		132.21	5, 495	0.930_4^{25}	1.5050^{25}	-1	170	26	s alc, eth

d245	Diethanolamine	HOCH ₂ CH ₂ NHCH ₂ CH ₂ OH	105.14	4, 283	1.088430	1.4747 ³⁰	28.0	268.0	137	96 aq; 4 bz; 0.8 eth; misc MeOH, acet
d246	2,2-Diethoxyaceto- phenone	$C_6H_5C(=O)CH (OC_2H_5)_2$	208.26	71, 361	1.034	1.4995 ²⁰		131- 134 ^{10mm}	110	
d247	4,4-Diethoxybutyl-	$H_2N(CH_2)_3CH$ (OC ₂ H ₅) ₂	161.25	4, 319	0.933	1.4275 ²⁰		196	62	
d248	2,2-Diethoxy- <i>N</i> , <i>N</i> -dimethylethylamine	(C ₂ H ₅ O) ₂ CHCH ₂ - N(CH ₃) ₂	161.25	4, 308	0.883	1.4129 ²⁰		170	45	
d249	Diethoxydimethyl- silane	$(C_2H_5O)_2Si(CH_3)_2$	148.28		0.840_4^{20}	1.3811 ²⁰	-87	114	11	
d250	Diethoxydiphenyl- silane	$(C_2H_5O)_2Si(C_6H_5)_2$	272.42		1.0329420	1.5269 ²⁰		130 ^{2mm}		
d251	1,1-Diethoxyethane	CH ₃ CH(OC ₂ H ₅) ₂	118.18	1,603	0.8254_4^{20}	1.3825^{20}	2.8	102.7	-21	5 ag; misc alc, eth
d252	1,2-Diethoxyethane	C ₂ H ₅ OCH ₂ CH ₂ OC ₂ H ₅	118.18	1,468	0.842	1.3922^{20}	-74	121.4	27	21 aq
d253	2,2-Diethoxyethanol	(C ₂ H ₂ O) ₂ CHCH ₂ OH	134.18	1,818	0.888^{24}_{4}	1.4160^{20}		167	67	s alc, eth
d254	2,2-Diethoxyethyl- amine	(C ₂ H ₅ O) ₂ CHCH ₂ NH ₂	133.19	4, 308	0.916	1.4170		162–163	45	
d255	Diethoxymethylsilane	$(C_2H_5O)_2SiH(CH_3)$	134.3		0.829_4^{25}	1.372^{25}		94–95		
d256	Diethoxymethylvinyl- silane	$(C_2H_5O)_2Si-$ $(CH_3)CH=CH_2$	160.3		0.858_4^{20}	1.400^{20}		133–134		
d257	1,1-Diethoxypropane	CH ₃ CH ₂ CH(OC ₂ H ₅) ₂	132.20	1,630	0.8232_4^{20}	1.3884^{20}		122.8	12	v s alc, eth
d258	3,3-Diethoxy-1-	$(C_2H_5O)_2CHCH=CH_2$	130.19	1,727	0.854	1.4000^{20}		89-90	4	
	propene									

 α ,p-Dichlorotoluene, c60

1,2-Dicyanoethane, b380



TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d259	2,2-Diethoxytri-	(C ₂ H ₅ O) ₂ CHCH ₂ N-	189.30	4, 309	0.850	1.418920		194–195	65	
d260	ethylamine N,N-Diethyl- acetamide	$(C_2H_5)_2$ $CH_3C(=O)N(C_2H_5)_2$	115.18	4, 110	0.925	1.4401 ²⁰		182–186	70	
d261	Diethyl acetamido- malonate	C ₂ H ₅ OOCCH(NHCOCH ₃)- COOC ₂ H ₅	217.22	4 ² , 891			97–98	185 ^{20mm}		
d262	Diethyl 1,3-acetone- dicarboxylate	C ₂ H ₅ OOCCH ₂ CO- CH ₂ COOC ₂ H ₅	202.21	3, 791	1.113	1.4385 ²⁰		250	86	
d263	Diethyl acetylenedi- carboxylate	$C_2H_5OOCC = CCOOC_2H_5$	170.16	2, 803	1.063	1.4426 ²⁰		107 ^{11mm}	94	
d264	Diethyl 2-acetyl- glutarate	C ₂ H ₅ OOCCH ₂ CH ₂ CH- (COCH ₃)COOC ₂ H ₅	230.26		1.071	1.4386 ²⁰		154 ^{11mm}	>112	
d265	Diethyl acetyl- succinate	C ₂ H ₅ OOCCH ₂ CH- (COCH ₃)COOC ₂ H ₅	216.23	3, 801	1.081	1.4346 ²⁰		180- 183 ^{50mm}	>112	
d266	Diethyl allyl- malonate	C ₂ H ₅ OOCCH(CH ₂ - CH=CH ₂)COOC ₂ H ₅	200.23	2,776	1.015	1.4304 ²⁰		222–223	92	
d267	Diethylamine	(C ₂ H ₅) ₂ NH	73.14	4, 95	0.7074_4^{20}	1.3864^{20}	-50.0	55.5	-28	misc aq, alc
d268	Diethylamine HCl	$(C_2H_5)_2NH \cdot HCl$	109.60	4, 95	1.048_4^{21}			320-330		s aq, alc, chl; i eth
d269	4-(Diethylamino)- benzaldehyde	$(C_2H_5)_2NC_6H_4CHO$	177.25	$14^2, 25$			39–41	174 ^{7mm}		
d270	2-Diethylamino- ethanol	(C ₂ H ₅) ₂ NCH ₂ CH ₂ OH	117.19	4, 282	0.8800 ²⁵	1.438925	-70	163	48	s aq, alc, bz, eth
d271	2-(Diethylamino)- ethyl-4-amino- benzoate	H ₂ NC ₆ H ₄ COOCH ₂ CH ₂ - N(C ₂ H ₅) ₂	236.30	14, 424			61			0.5 aq; s alc, bz, eth
d272	2-Diethylaminoethyl chloride HCl	$CICH_2CH_2N(C_2H_5)_2 \cdot HCI$	172.10	$4^2,618$			208–210			
d273	3-(Diethylamino)- phenol	$(C_2H_5)_2NC_6H_4OH$	165.24	13, 408			65–69	170 ^{15mm}		s aq, alc, eth

d274	3-Diethylamino-1,2-	$(C_2H_5)_2NCH_2CH(OH)$ -	147.22	4, 302	0.973_{20}^{20}	1.4602^{20}	233–235		107	s aq, alc, chl, eth
	propanediol	CH₂OH								
d275	1-Diethylamino-2-	$(C_2H_5)_2NCH_2CH(OH)$ -	131.22	4^2 , 737	0.889	1.4255^{20}	13.5	55-59 ^{13mm}	33	s alc
	propanol	CH_3								
d276	4-(Diethylamino)- salicylaldehyde	$(C_2H_5)_2NC_6H_3(OH)CHO$	193.25	14, 234			62–64			
d277	N, N-Diethylaniline	$C_6H_5N(C_2H_5)_2$	149.24	12, 164	0.9302_4^{25}	1.539425	-34.4	216.3	97	1 aq; sl s alc, eth
d278	2,6-Diethylaniline	$(C_2H_5)_2C_6H_3NH_2$	149.24		0.906	1.5452^{20}	3	243	123	
d279	Diethyl azodicar-	$C_2H_5OOCN = NCOOC_2H_5$	174.16	3, 123	1.106	1.4280^{20}		106 ^{13mm}	26	
	boxylate									
d280	5,5-Diethylbar-		184.19	$24^2, 279$	1.220		188-192			0.7 aq; 7 alc; 1.3
	bituric acid									chl; 3.2 eth; s
										acet, HOAc
d281	Diethyl benzal-	$C_6H_5CH = C(COOC_2H_5)_2$	248.28	9, 892	1.107	1.5365^{20}		215 ^{30mm}	>112	
	malonate									
d282	1,2-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8800^{20}	1.5022^{20}	-31.3	183.4	49	s alc, eth
d283	1,3-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8640_4^{20}	1.4950^{20}	-83.9	181.1	50	s alc, eth
d284	1,4-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8620_4^{20}	1.4940^{20}	-42.85	183.8	56	s alc, eth
d285	Diethyl benzyl-	C ₆ H ₅ CH ₂ CH-	250.29	9, 869	1.064	1.4868^{20}		162 ^{10mm}	>112	
	malonate	$(COOC_2H_5)_2$								
d286	Diethyl bromo-	BrCH(COOC ₂ H ₅) ₂	239.07	2, 594	1.4022_4^{25}	1.4550^{20}	-54	233-235 d		i aq; misc alc, eth
	malonate									

Diethyl acetal, d251 Diethylacetic acid, e89 Diethyl 2-acetylpentanedioate, d264 Diethylaminoacetaldehyde diethyl acetal, d259 3-Diethylaminopropylamine, d330 Diethyl (*Z*)-2-butenedioate, d316

$$C_2H_5$$
 C_2H_5
 C_2H_5
 C_2H_5
 C_2H_5
 C_2H_5

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d287	Diethyl butyl- malonate	C ₄ H ₉ CH(COOC ₂ H ₅) ₂	216.28	21, 282	0.983	1.4220		235–240	93	v s alc, eth
d288	Diethylcarbamoyl chloride	(C ₂ H ₅) ₂ NCOCl	135.59	4, 120		1.4515 ²⁰		187–190	75	d hot aq, hot alc
d289	Diethyl carbonate	$(C_2H_5O)_2C=O$	118.13	3, 5	0.9764_4^{20}	1.3843 ²⁰	-43.0	126.8	25	69 aq; misc alc, bz, eth, esters
d290	Diethyl chloro- malonate	CICH(COOC ₂ H ₅) ₂	194.61	$2^2,537$	1.2040_4^{20}	1.4310^{20}		222–223		misc alc, chl, eth
d291	Diethyl chloro- phosphate	$(C_2H_5O)_2P(O)Cl$	172.55	1, 332	1.194	1.4165 ²⁰		60 ^{2mm}		
d292	Diethyl chloro- thiophosphate	$(C_2H_5O)_2P(S)Cl$	188.61		1.200	1.4715 ²⁰		45 ^{3mm}		
d293 d293a	Diethylcyanamide Diethyl cyanomethyl- phosphonate	(C ₂ H ₅) ₂ NCN (C ₂ H ₅ O) ₂ P(O)CH ₂ CN	98.15 177.14	4, 121	0.846 1.095	$ \begin{array}{c} 1.4229^{20} \\ 1.4312^{20} \end{array} $		186–188 101 ^{0.4mm}	69 >112	
d294	N,N-Diethylcyclo- hexylamine	$C_6H_{11}N(C_2H_5)_2$	155.29	12, 6	0.850	1.456220		194–195	57	
d294a	Diethyl disulfide	C ₂ H ₅ SSC ₂ H ₅	122.25	1, 347	0.998_4^{20}	1.506320	-101.5	154.0		sl s aq; misc alc, eth
d295	Diethyldithio- carbamic acid, Na salt	$ \begin{array}{c} (C_2H_5)_2NC(=S)S^-Na^+ \cdot \\ 3H_2O \end{array} $	225.31	4 ² , 613			95–99			
d296	Diethyl dithio- phosphate	$(C_2H_5O)_2P(S)SH$	186.23	1, 333	1.111	1.5120 ²⁰		60 ^{1mm}		
d297	N, N-Diethyldodecan- amide	$CH_3(CH_2)_{10}C(O)N (C_2H_5)_2$	255.45		0.847	1.4545 ²⁰		166 ^{2mm}	>112	
d298	Diethylenetriamine	(H ₂ NCH ₂ CH ₂) ₂ NH	103.17	4, 255	0.9542_{20}^{20}	1.4826 ²⁰	-35	207.1	101	misc aq, alc, bz, eth

d299	Diethylenetriamine-	[(HOOCCH ₂) ₂ NCH ₂ -	393.35				220 d			
d300	pentaacetic acid Diethyl ether	CH ₂] ₂ NCH ₂ COOH C ₂ H ₅ OC ₂ H ₅	74.12	1,314	0.7134_4^{20}	1.3527 ²⁰	-116.3	34.6	-40	6 aq; misc alc, bz,
d301	Diethyl ethoxymethyl- enemalonate	(C ₂ H ₅ OOC) ₂ C=CH- OC ₂ H ₅	216.23	3, 469	1.070	1.4620^{20}		279–281	155	chl
d302	N,N-Diethylethyl- enediamine	$(C_2H_5)_2NCH_2CH_2NH_2$	116.21	4,251	0.827	1.4360^{20}		145–147	30	
d303	Diethyl ethyl- malonate	C ₂ H ₅ CH(COOC ₂ H ₅) ₂	188.2	2,644	1.004_{20}^{20}	1.4158^{20}		75–77 ^{5mm}	88	sl s aq; v s alc, eth
d304	N,N-Diethyl- formamide	$(C_2H_5)_2NCHO$	101.15	4, 109	0.908	1.4340^{20}		176–177	60	misc aq; v s alc,
d305	Diethyl fumarate	C ₂ H ₅ OOCCH=CH- COOC ₃ H ₅	172.18	2,742	1.052_4^{20}	1.4406^{20}	1–2	218–219	91	Cui
d306	Diethyl 3,4-furandi- carboxylate	$(C_2H_5OOC)_2C_4H_2O$	212.20		1.140	1.4717^{20}		155 ^{13mm}	82	
d307	Diethyl glutarate	C ₂ H ₅ OOCCH ₂ CH ₂ CH ₂ - COOC ₂ H ₅	188.22	2, 633	1.022	1.4240^{20}	-23.8	237	96	0.9 aq; v s alc; s eth
d308	2,4-Diethyl-2,6- heptadienal	$H_2C = CHCH_2CH(C_2H_5)$ - $CH = C(C_2H_5)CHO$	166.27					91 ^{12mm}		
d309	Diethyl heptane- dioate	C ₂ H ₅ OOC(CH ₂) ₅ - COOC ₂ H ₅	216.28	2, 671	0.9945 ²⁰	1.4280^{20}	-24	192 ^{100mm}	>112	i aq; s alc, eth
d310	2,4-Diethyl-1- heptanol	CH ₃ CH ₂ CH ₂ CH(C ₂ H ₅)- CH ₂ CH(C ₂ H ₅)CH ₂ OH	172.31					109 ^{12mm}		

Diethyl carbitol, b176
Diethylene dioxide, d646
Diethylene glycol, b181
Diethylene glycol dibutyl ether, b151
Diethylene glycol diethyl ether, b176
Diethylene glycol dimethyl ether, b191

Diethylene glycol monobutyl ether, b411 Diethylene glycol monoethyl ether, e35 Diethylene glycol monoethyl ether acetate, e36 Diethylene glycol monomethyl ether, m66 Diethyleneimide oxide, m448 Diethyl ethoxycarbonylmethylphosphonate, t283

N,N-Diethylethanamine, t264

N,N-Diethylethanolamine, d270

Di-2-ethylhexyl adipate, d312

Di-2-ethylhexyl sebacate, d311

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d311	Di-(2-ethylhexyl) decanedioate	C ₄ H ₉ CH(C ₂ H ₅)CH ₂ OOC- (CH ₂) ₈ COOCH ₂ CH- (C ₂ H ₅)C ₄ H ₉	426.68		0.912425	1.451 ²⁵		256 ^{5mm}	227	i aq; s alc, bz, acet
d312	Di-(2-ethylhexyl) hexanedioate	C ₄ H ₉ CH(C ₂ H ₅)CH ₂ OOC- (CH ₂) ₄ COOCH ₂ CH- (C ₂ H ₅)C ₄ H ₉	370.57		0.925_{25}^{25}	1.4474 ²⁰		214 ^{5mm}	193	s alc, eth, acet; iaq
d313	Di-(2-ethylhexyl) <i>o</i> -phthalate	$C_6H_4[COOCH_2CH-(C_2H_5)C_4H_9]$	390.56		0.981_{25}^{25}	1.4853 ²⁰	-50	384	207	
d314	Diethyl hydrogen phosphonate	$(C_2H_5O)_2P(O)H$	138.10	1, 330	1.079_4^{20}	1.4076 ²⁰		50-51 ^{2mm}	90	s aq (hyd), alc, eth
d315	N,N-Diethylhydroxyl- amine	$(C_2H_5)_2NOH$	89.14	4, 536	1.867	1.4195 ²⁰	-25	125–130	45	
d316	Diethyl maleate	C ₂ H ₅ OOCCH=CH- COOC ₂ H ₅	172.18	2,751	1.0687 ²⁰	1.4400 ²⁰	-8.8	225.3	93	1.4 aq; s alc, eth
d317	Diethyl malonate	C ₂ H ₅ OOCCH ₂ COOC ₂ H ₅	160.17	2, 573	1.0550	1.4136 ²⁰	-48.9	199.3	100	2.7 aq; misc alc, eth
d318	Diethylmalonic acid	HOOCC(C ₂ H ₅) ₂ COOH	160.17	2,686			127	d 170-180		v s aq, alc, eth
d319	<i>N,N</i> -Diethyl-3- methylbenzamide	$CH_3C_6H_4C(=O)N-(C_2H_5)_2$	191.27	$9^2,325$	0.996_4^{20}	1.521220		111 ^{1mm}		s aq; v s alc, bz, eth
d320	Diethyl methyl- malonate	C ₂ H ₅ OOCCH(CH ₃)- COOC ₂ H ₅	174.20	2, 629	1.018_4^{20}	1.4130 ²⁰		198	76	sl s aq; v s alc, eth
d321	Diethyl 2-methyl-2'- oxosuccinate	$C_2H_5OOCCH(CH_3)-$ $C(=O)C(=O)OC_2H_5$	202.21	3, 794	1.073	1.4313 ²⁰		138 ^{23mm}	>112	
d322	Diethyl methyl- succinate	C ₂ H ₅ OOCCH ₂ CH(CH ₃)- COOC ₃ H ₅	188.22	2, 639	1.012	1.4199 ²⁰		217–218		
d323	N,N-Diethyl-4- nitrosoaniline	$C_6H_4(NO)N(C_2H_5)_2$	178.24	12, 684			82–84			
d324	Diethyl octanedioate	C ₂ H ₅ OOC(CH ₂) ₆ - COOC ₂ H ₅	230.30	2, 693	0.9822_4^{20}	1.4323 ²⁰	5.9	282	>112	i aq; s alc, eth

d325	Diethyl oxalate	C ₂ H ₅ OOCCOOC ₂ H ₅	146.14	2, 535	1.0785_4^{20}	1.4102	-40.6	185.4	75	3.6aq (gradual d); misc alc, eth
d326	Diethyl oxydiformate	$[C_2H_5OC(=O)]_2O$	162.14		1.12420	1.3980^{20}		93 ^{18mm}	69	s alc, esters, ketones
d327	N ¹ ,N ¹ -Diethyl-1,4- pentanediamine	CH ₃ CH(NH ₂)(CH ₂) ₃ - N(C ₂ H ₅) ₂	158.29		0.817	1.4429^{20}		200 ^{753mm}	68	s aq, alc, eth
d328	Diethyl phenyl- malonate	$C_6H_5CH(COOC_2H_5)_2$	236.27	9, 854	1.0950_4^{20}	1.4913^{20}	16	170 ^{14mm}	>112	i aq; s alc
d329	Diethyl o-phthalate	$C_6H_4(COOC_2H_5)_2$	222.24	9, 798	1.23214	1.5049^{14}	-3	295	140	i aq; misc alc, eth
d330	N,N-Diethyl-1,3- propanediamine	(C ₂ H ₅) ₂ NCH ₂ CH ₂ - CH ₂ NH ₂	130.24		0.826	1.4416^{20}		159	58	,
d331	2,2-Diethyl-1,3- propanediol	$(C_2H_5)_2C(CH_2OH)_2$	132.20		1.05220	1.4574 ²⁵	61.3	125 ^{10mm}		25 aq; v s alc, eth
d332	Diethyl propyl- malonate	$C_2H_5OOCCH(C_3H_7)-COOC_3H_5$	202.25	2,657	0.987	1.4185^{20}		221–222	91	
d333	1,1-Diethyl-2- propynylamine	$HC \equiv CC(C_2H_5)_2NH_2$	111.19		0.828	1.4409^{20}		71 ^{90mm}	21	
d334	N,N-Diethyl-3- pyridine- carboxamide	$C_5H_4N-C(=O)N-(C_2H_5)_2$	178.24	22 ² , 34	1.060425	1.5240 ²⁰	24–26	296–300	>112	
d335	Diethyl succinate	C ₂ H ₅ OOCCH ₂ CH ₂ - COOC ₂ H ₅	174.20	2, 609	1.040_4^{20}	1.4200^{20}	-21	217.7	110	i aq; misc alc, eth
d336	Diethyl sulfate	$(C_2H_5O)_2SO_2$	154.18	1, 327	1.172_4^{25}	1.4004^{20}	-25	209 d	78	misc alc, eth
d337	Diethyl sulfide	$(C_2H_5)_2S$	90.19	1,344	0.8367_4^{20}	1.4430^{20}	-103.9	92.1	-9	i aq; misc alc, eth
d338	Diethyl sulfite	$(C_2H_5O)_2S(O)$	138.19	1,325	1.077_4^{25}			157.7		s aq(d), alc

Diethyl ketone, p42 *N,N*-Diethylnicotinamide, d334 *O,O*-Diethyl *O-p*-nitrophenyl phosphorothioate, p3 Diethyl 3-oxoglutarate, d262 Diethyl 2-pentenedioate, d307 Diethyl phosphite, d314 Diethyl phosphorochloridate, d291 Diethyl phosphorochloridothionate, d292 Diethyl pimelate, d309

Diethyl propanedioate, d317 1,1-Diethyl propargylamine, d333 Diethyl pyrocarbonate, d326 Diethyl suberate, d324

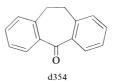
TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d339	(+)-Diethyl-	[—CH(OH)COOC ₂ H ₅] ₂	206.19	3, 512	1.20420	1.4459 ²⁰	17	280	93	sl s aq; misc alc, eth
d340	L-tartrate (-)-Diethyl- D-tartrate	[—CH(OH)COOC ₂ H ₅] ₂	206.19	31, 181	1.205	1.4467 ²⁰		162 ^{19mm}	93	
d341	Diethyl 3,3'-thio- propionate	S(CH ₂ CH ₂ COOC ₂ H ₅) ₂	234.32		1.095	1.4655 ²⁰		121 ^{2mm}		
d342	N,N-Diethyl-m- toluamide	$CH_3C_6H_4C(=O)N (C_2H_5)_2$	191.27	$9^2,325$	0.996	1.521220		111 ^{1mm}		
d343	N,N-Diethyl-1,1,1- trimethylsilyl- amine	$(C_2H_5)_2NSi(CH_3)_3$	145.32		0.767	1.408120		125–126	10	
d344	Diethylzinc	$(C_2H_5)_2Zn$	123.49		1.206520		-28	118		
d345	1,4-Difluorobenzene	$C_6H_4F_2$	114.09	5, 199	1.1701^{20}	1.441520	-23.7	88.9	2	
d346	1,1-Difluoroethane	CH ₃ CHF ₂	66.05	3, 177	0.909^{21}	1.4413	-117	-24.7	_	0.32 ag
d347	1,1-Difluorotetra-	Cl ₃ CCClF ₂	203.83	1,86	1.649	1.413	41	91	none	sl s alc; v s eth
u5 17	chloroethane	C13CCCH 2	203.03	1,00	1.017	1.115		'	none	Si S die, v S edi
d348	1,2-Difluorotetra- chloroethane	FCl ₂ CCCl ₂ F	203.83	1 ³ , 365	1.6447425	1.413 ²⁵	23.8	203.8		i aq; s alc, eth
d349	Dihexylamine	$(C_6H_{13})_2NH$	185.36	4 ¹ , 384	0.795	1.4320^{20}		192-195	95	s alc, eth
d350	Dihexyl ether	$(C_6H_{13})_2O$	186.34	1 ³ , 1656	0.7936_4^{20}	1.4204^{20}		226.2	77	i aq; s eth
d351	9,10-Dihydro- anthracene		180.25	5, 641	0.880		108–110	312		i aq; s alc, bz, eth
d352	(+)-Dihydrocarvone		152.24	$7^3,337$	0.929^{19}	1.4718^{20}		221–222	81	
d353	Dihydrocoumarin		148.16	17, 315	1.169^{18}	1.556320	25	272		sl s alc, eth; s chl
d354	10,11-Dihydro-5 <i>H</i> -		208.26		1.156	1.6332^{20}	32–34	148 ^{0.3mm}	>112	, ,
	dibenzo-[a,d]cyclo-									
	hepten-5-one									
d355	3,4-Dihydro-2-		128.17		0.957	1.4394^{20}		42 ^{16mm}	24	
	ethoxy-2 <i>H</i> -pyran									

d356	2,3-Dihydrofuran		70.09	17 ³ , 141	0.927	1.4239^{20}		54-55	<1	
d537	Dihydrolinalool	(CH ₃) ₂ C=CHCH ₂ CH ₂ -	156.27		0.925^{25}	1.433^{20}			178	
		C(OH)(CH ₃)CH ₂ CH ₃								
d358	3,4-Dihydro-1(2 <i>H</i>)-		176.22	$9^2,889$			80	171 ^{11mm}		
	6-methoxynaphtha-									
	lenone									
d359	3,4-Dihydro-2-		114.14			1.4425^{20}			16	
	methoxy-2H-pyran									
d360	2,3-Dihydro-2-		134.18	171, 23	1.061	1.5308^{20}		197-198	62	
	methylbenzofuran									
d361	5,6-Dihydro-4-		98.15	17 ³ , 160	0.912	1.4495^{20}		117-118	21	
	methyl-2 <i>H</i> -pyran									

Diglycine, i10 Diglycol, b181 Diglycolic acid, o61 Diglyme, b191 Dihydroanisoles, m61, m62 6,7-Dihydro-5*H*-cyclopenta[b]pyridine, c360 10,11-Dihydro-5*H*-dibenz[*b,f*]acepine, i12 2,5-Dihydro-2,5-dimethoxyfuran, d436 3,7-Dihydro-3,7-dimethyl-1*H*-pyridine-2,6-dione, t138
2,3-Dihydroindene, i13
Dihydromyrcenol, m303

d353



d355

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d362	3,4-Dihydro-1(2 <i>H</i>)-		146.19	7, 370	1.099	1.568520	5–6	116 ^{6mm}	>112	
	naphthalenone									
d363	Dihydropyran		84.12		0.922_{15}^{19}	1.4410^{20}	-70	86	-15	s aq, alc
d364	5,6-Dihydro-2 <i>H</i> -		112.13		1.100	1.4980^{20}		78 ^{12mm}	77	
	pyran-3-carbal-									
	dehyde									
d365	3,4-Dihydro-2 <i>H</i> -		150.11				242–244			
	pyran-2-carboxylic									
	acid, Na salt				25	= 0.00				
d366	Dihydroterpineol		256.27		0.907^{25}	1.4670 ²⁰		. 0 17	88	
d367	5,6-Dihydro-2,4,4,6-		141.21		0.886	1.4410^{20}		48 ^{17mm}		
	tetramethyl-4H-									
1270	1,3-oxazine 2,5-Dihydrothio-		118.15				64–66		>112	1-11-1
d368	phene-1,1-dioxide		118.15				04-00		>112	s aq, alc, bz, chl, eth
d369	1,2-Dihydro-2,2,4-		173.26		0.934	1.589520		90 ^{0.02mm}	101	Cui
u309	trimethylquinoline		173.20		0.934	1.3693		90	101	
d370	2',4',-Dihydroxyacet-	$(HO)_2C_6H_3C(=O)CH_3$	152.15	8, 266	1.180		145–147			s warm alc, pyr,
u 370	ophenone	(110)2061130(-0)0113	132.13	0, 200	1.100		143 147			HOAc; i bz, chl,
	opiiciione									eth
d371	1,2-Dihydroxyanthra-		240.21	8, 439			287–289	430		s alc, bz, chl,
	quinone									HOAc
d372	1,4-Dihydroxyanthra-		240.21	8,450			196			s alc, alk, eth
	quinone									
d373	1,8-Dihydroxyanthra-		240.21	8, 458			193-197	subl		0.005 alc; 0.2 eth;
	quinone									s chl
d374	2,6-Dihydroxyanthra-		240.21	8, 463			360 d			sl s aq, alc
	quinone									
d375	2,4-Dihydroxybenz-	(HO) ₂ C ₆ H ₃ CHO	138.12	8, 241			135–136	226 ^{22mm}		v s aq, alc, chl, eth
	aldehyde									

d376	3,4-Dihydroxybenz- aldehyde	(HO) ₂ C ₆ H ₃ CHO	138.12	8, 246		153			5 aq; 79 hot alc; v
d377	1,2-Dihydroxybenzene	$C_6H_4(OH)_2$	110.11	6, 759	1.344 ⁴	104–106	245.5	137	43 aq; s alc, bz, chl, eth; v s pyr,
d378	1,3-Dihydroxybenzene	C ₆ H ₄ (OH) ₂	110.11	6 ² , 802	1.27215	109–110	276	171	alk 110 aq; 110 alc; v s eth, glyc; sl s chl
d379	1,4-Dihydroxybenzene	$C_6H_4(OH)_2$	110.11	6,836	1.33215	170–171	285–287		7 aq; v s alc, eth

4,5-Dihydro-2-(phenylmethyl)-1H-imidazole, b102

Dihydroresorcinol, c322

3,7-Dihydro-1,3,7-trimethyl-1*H*-purine-2-6-dione, c1

1,3-Dihydroxyacetone, d397

2,2'-Dihydroxy-2,2'-biindan-1,2',3,3'tetrone, h85

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d380	1,3-Dihydroxybenzene	HOC ₆ H ₄ OOCCH ₃	152.15	6, 816		1.5350 ²⁰		283	>112	
d381	monoacetate 2,5-Dihydroxy-p- benzenedisulfonic acid, K salt	$(HO)_2C_6H_2(SO_3^-K^+)_2$	346.43	11,300			>300			v s aq
d382	2,5-Dihydroxy- benzenesulfonic acid, K salt	$(HO)_2C_6H_3SO_3^-K^+$	228.27	11,300			251 d			v s aq
d383	2,4-Dihydroxybenzoic	(HO) ₂ C ₆ H ₃ COOH	154.12	10, 377			213			s hot aq, alc, eth
d384	2,5-Dihydroxybenzoic	(HO) ₂ C ₆ H ₃ COOH	154.12	10, 384			199–200			0.5 aq; s alc, eth
d385	3,5-Dihydroxybenzoic	(HO) ₂ C ₆ H ₃ COOH	154.12	10, 404			236 d			sl s aq; s alc, eth
d386	2,4-Dihydroxybenzo- phenone	$(HO)_2C_6H_3C(=O)C_6H_5$	214.22	8, 312			144–145			v s alc, eth, HOAc
d387	2,2'-Dihydroxybi- phenyl	HOC ₆ H ₄ C ₆ H ₄ OH	186.21	6, 989			110	315		s alc, bz, eth; sl s
d388	4,6-Dihydroxy-2- mercaptopyrimidine		144.15	24, 476			236			uq
d389	1,2-Dihydroxy-4- methylbenzene	$(HO)_2C_6H_3CH_3$	124.14	6, 878	1.1294	1.5425 ⁷⁴	67–69	251		v s aq, alc, eth
d390	1,3-Dihydroxy-2- methylbenzene	$(HO)_2C_6H_3CH_3$	124.14	6, 878			115–118	264		s aq, alc, bz, eth
d391	2,4-Dihydroxy-6- methylpyrimidine		126.12	24, 342			318 d			
d392	1,5-Dihydroxynaph- thalene	C ₁₀ H ₆ (OH) ₂	160.17	6,980			259 d			sl s aq; s alc; v s eth

d393	1,7-Dihydroxynaph-	$C_{10}H_6(OH)_2$	160.17	6,981		177–180			v s alc, eth
	thalene								
d394	2,3-Dihydroxynaph-	$C_{10}H_6(OH)_2$	160.17	6, 982		162-164			v s alc, eth
	thalene	-106()2		-,,,,,					
1205		C H (OH)	160.17	6.005		107.1			1 1 1
d395	2,7-Dihydroxynaph-	$C_{10}H_6(OH)_2$	160.17	6, 985		187 d			sl s aq; v s alc, eth
	thalene								
d396	4,5-Dihydroxynaph-	$(HO)_2C_{10}H_4(SO_3H)_2$	296.26	11, 307					v s aq; i alc, eth
	thalene-2.7-								_
	disulfonic acid								
1207		HOCH C(O)CH OH	00.00	1 046		65–71			
d397	1,3-Dihydroxy-2-	$HOCH_2C(=O)CH_2OH$	90.08	1,846		03-71			v s aq, alc, acet,
	propanone								eth
d398	2,3-Dihydroxy-	HOCH₂CHOCHO	90.08	1,845	1.455_{18}^{18}	145	140 ^{0.8mm}	>112	3 aq; i bz, PE
	propionaldehyde								_
d399	7-(2,3-Dihydroxy-		254.25			158			33 aq; 2 alc; 1 chl
4377	propyl)theophylline		23 1.23			150			33 44, 2 410, 1 6111
1400	1 10 / 10		112.00	24 212		1260			
d400	3,6-Dihydroxy-		112.09	24, 312		d 260			sl s hot alc; s hot
	pyridazine								aq
d401	2,3-Dihydroxy-	(HO) ₂ C ₅ H ₃ N	111.10	21^2 , 107		245 d			
	pyridine								

2,2'-Dihydroxydiethylamine, d245 *N*,*N*-Di(hydroxyethyl)aminoacetic acid, b182 2,2-Dihydroxy-1,3-indandione, i16

2,2-Dihydroxymethyl-1-butanol, e156 1,8-Dihydroxynaphthalene-3,6-disulfonic acid, d396 Dihydroxypropanes, p194, p195

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d402 d403 d404	1,4-Diiodobenzene 1,2-Diiodoethane Diiodomethane	C ₆ H ₄ I ₂ ICH ₂ CH ₂ I CH ₂ I ₂	329.91 281.86 267.84	5, 227 1, 99 1, 71	$\begin{array}{c} 2.132^{10} \\ 3.325_4^{20} \end{array}$	1.7411 ²⁰	131–133 81 5.6	285 200 181		sl s alc; v s eth sl s aq; s alc, eth 0.12 aq; misc alc, bz, eth, PE
d405 d406	1,3-Diiodopropane Diisobutylamine	ICH ₂ CH ₂ CH ₂ I [(CH ₃) ₂ CHCH ₂] ₂ NH	295.88 129.25	1, 115 4, 166	2.5755 ²⁰ 0.740	1.6423 ²⁰ 1.4081 ²⁰	-13 -77	222 137–139	29	i aq; s chl, eth s alc, acet, eth, EtAc
d407 d408	Diisobutyl ether Diisobutyl hexanedioate	[(CH ₃) ₂ CHCH ₂] ₂ O [(CH ₃) ₂ CHCH ₂ OOC- CH ₂ CH ₂ —] ₂	130.22 258.36		$0.761^{15} \\ 0.950^{25}_{25}$			122–124	160	i aq; misc alc, eth
d409	Diisobutyl- o-phthalate	$C_6H_4[COOCH_2CH-(CH_3)_2]_2$	278.35		1.038_{25}^{25}				174	
d410	1,6-Diisocyanato- hexane	OCN(CH ₂) ₆ NCO	168.20	$4^2,711$	1.040	1.4525 ²⁰		255	140	
d411	Diisopropylamine	[(CH ₃) ₂ CH] ₂ NH	101.19	4, 154	0.7169^{20}	1.392420	-96.3	83.5	-6	11 aq
d412	2-(Diisopropylamino)- ethanol	[(CH ₃) ₂ CH] ₂ NCH ₂ - CH ₂ OH	145.25	41, 430	0.826	1.4417 ²⁰		187–192	57	
d413	2,6-Diisopropyl- aniline	[(CH ₃) ₂ CH] ₂ C ₆ H ₃ NH ₂	177.29	12, 168	0.940	1.533220	-45	257	123	
d414	1,3-Diisopropyl- benzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	5, 447	0.856_4^{20}	1.4980^{20}	-63	203	76	misc alc, bz, eth,
d415	1,4-Diisopropyl- benzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	$5^2,339$	0.857_4^{20}	1.4889 ²⁰		203	76	misc alc, bz, eth,
d416	Diisopropyl- cyanamide	[(CH ₃) ₂ CH] ₂ NCN	126.20	$4^3, 279$	0.839	1.4270^{20}		93 ^{25mm}	78	
d417	Diisopropyl ether	[(CH ₃) ₂ CH] ₂ O	102.17	1, 362	0.7258_4^{20}	1.3689 ²⁰	-86.9	68.4	-12	1.2 aq; misc alc, bz, chl, eth
d418	N,N-Diisopropyl- ethylamine	[(CH ₃) ₂ CH] ₂ NC ₂ H ₅	129.25		0.742	1.4133 ²⁰		127	10	52, 511, 511

d419	2,6-Diisopropyl-	[(CH ₃) ₂ CH] ₂ C ₆ H ₃ OH	178.28	$6^1, 272$	0.962	1.5140^{20}	18	256	>112	l
	phenol	12 - 3/2 - 3/2 - 6 3 -								
d420	Diisopropyl	$[(CH_3)_2CHO]_2P(O)H$	166.16	1, 363	0.997	1.4070^{20}		72-75 ^{10mm}	>112	
	phosphite									
d421	(+)-Diisopropyl	[—CH(OH)COOCH-	234.25	3,517	1.114	1.4387^{20}		152 ^{12mm}	109	
	L-tartrate	$(CH_3)_2]_2$								
d422	Diketene		84.07		1.073	1.4330^{20}		127	33	
d423	Dilauryl phosphite	$[CH_3(CH_2)_{11}O]_2P(O)H$	418.64		0.946	1.4520^{20}			>112	
d424	threo-1,4-Dimercapto-	HSCH ₂ CH(OH)CH(OH)-	154.25				42–43			v s aq, alc, chl, eth
	2,3-butanediol	CH ₂ SH								
d425	2,3-Dimercapto-1-	HSCH ₂ CH(SH)CH ₂ OH	124.22		1.2385_4^{25}	1.5720^{25}		120 ^{15mm}	>112	8 aq(d); s alc, eth
	propanol									
d426	3',4'-Dimethoxyacet-	$(CH_3O)_2C_6H_3COCH_3$	180.20	$8^2,298$			49–51	286–288		sl s aq, alc, eth
	ophenone									
d427	2,4-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 784			34–37			s alc, bz, eth
d428	2,5-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 788			80–82	270 sl d		s aq, alc
d429	3,4-Dimethoxyaniline	$(CH_3O)_2C_6H_3NH_2$	153.18	13, 780			88	176 ^{22mm}		s hot eth
d430	3,4-Dimethoxybenz-	$(CH_3O)_2C_6H_3CHO$	166.18	8, 255			42–43	281		v s alc, eth
	aldehyde									
d431	1,2-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6,771	1.0819^{25}	1.5232^{25}	22.5	206.3	87	sl s aq; s alc, eth
d432	1,3-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6,813	1.055	1.5240	-55	85–87 ^{7mm}	87	s alc, bz, eth; sl s
										aq
d433	1,4-Dimethoxybenzene	$C_6H_4(OCH_3)_2$	138.17	6, 843	1.036_4^{68}		55-60	213		s alc; v s bz, eth

Dihydroxytoluene, d390 3, 5-Diiodosalicylic acid, h111 2Diisobutyl adipate, d408 Diisobutylene, t357 Diisobutyl ketone, d531 Diisopropyl ketone, d578 Diisopropylmethane, d572 Dimedone, d508 1, 1-Dimethoxytrimethylamine, d523

$$CH_2 = C - O$$

$$CH_2 - C = O$$

$$d422$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d434	3,4-Dimethoxybenzoic	(CH ₃ 0) ₂ C ₆ H ₃ COOH	182.18	10¹, 188			180–181			0.047 aq; v s alc,
d435	1,1-Dimethoxy-3- butanone	(CH ₃ O) ₂ CHCH ₂ COCH ₃	132.16		0.993	1.4150 ²⁰			49	
d436	2,5-Dimethoxy-2,5- dihydrofuran		130.14		1.073	1.4339 ²⁰		160–162	47	
d437	Dimethoxydiphenyl-silane	$(C_6H_5)_2Si(OCH_3)_2$	244.4		1.0771_4^{20}	1.5447 ²⁰		161 ^{15mm}		
d438	1,1-Dimethoxyethane	CH ₃ CH(OCH ₃) ₂	90.12	1,603	0.8502^{20}		-113	64.5		s aq, alc, chl, eth
d439	1,2-Dimethoxyethane	CH ₃ OCH ₂ CH ₂ OCH ₃	90.12	1,467	0.8629_4^{20}	1.3796^{20}	-68	85.2	1	misc aq, alc; s PE
d440	(2,2-Dimethoxy)- ethylamine	H ₂ NCH ₂ CH(OCH ₃) ₂	105.14	$4^2,758$	0.965	1.4170^{20}		135 ^{95mm}	53	_
d441	Dimethoxymethane	CH ₂ (OCH ₃) ₂	76.10	1,574	0.8601_{20}^{20}	1.3534^{20}	-104.8	42.3	-17	32 aq
d442	1,1-Dimethoxy-2- methylaminoethane	CH ₃ NHCH ₂ CH(OCH ₃) ₂	119.16	$4^2,759$	0.928	1.4115 ²⁰		140	29	
d443	Dimethoxymethyl- phenylsilane	(CH ₃ O) ₂ Si(CH ₃)C ₆ H ₅	182.3		0.993_4^{20}	1.469 ²⁰		199–200		
d444	1,2-Dimethoxy-4- nitrobenzene	$(CH_3O)_2C_6H_3NO_2$	183.16	6, 789	1.1888433		95–98	230 ^{17mm}		v s alc, eth; s chl
d445	2,5-Dimethoxy-4'- nitrostilbene	$(CH_3O)_2C_6H_3CH$ = CH - $C_6H_4NO_2$	285.30	6 ² , 987			117–119			
d446	2,6-Dimethoxyphenol	(CH ₃ O) ₂ C ₆ H ₃ OH	154.17	6, 1081			53-56	261		s alc, alk; v s eth
d447	(3,4-Dimethoxy)- phenylacetic acid	(CH ₃ O) ₂ C ₆ H ₃ CH ₂ COOH	196.20	10, 409			96–98			s aq; v s alc, eth
d448	(3,4-Dimethoxy)- phenylacetonitrile	(CH ₃ O) ₂ C ₆ H ₃ CH ₂ CN	177.20	10 ¹ , 198			62–63	171- 178 ^{10mm}		
d449	2,2-Dimethoxy-2- phenylacetophenone	$ \begin{array}{c c} C_6H_5C(O)C(OCH_3)_2 - \\ C_6H_5 \end{array} $	256.30				67–70			

d450	1,1-Dimethoxy-2- phenylethane	C ₆ H ₅ CH ₂ CH(OCH ₃) ₂	166.22	7, 293	1.004	1.4950^{20}		221	83	
d451	β -(3,4-Dimethoxy)-phenylethylamine	(CH ₃ O) ₂ C ₆ H ₃ CH ₂ - CH ₂ NH ₂	181.24	13, 800	1.074	1.5464 ²⁰		188 ^{15mm}		
d452	2,2-Dimethoxy- propane	(CH ₃) ₂ C(OCH ₃) ₂	104.15	1,648	0.847	1.3780		83	4	
d453	1,1-Dimethoxy-2- propanone	CH ₃ C(O)CH(OCH ₃) ₂	118.13	1 ¹ , 395	0.976	1.3978 ²⁰		143–147	37	
d454	3,3-Dimethoxy-1- propene	(CH ₃ O) ₂ CHCH=CH ₂	102.13	11, 378	0.862	1.3954 ²⁰		89–90		
d455	1,2-Dimethoxy-4- propenylbenzene	$CH_3CH = CHC_6H_3$ - $(OCH_3)_2$	178.23	6, 956	1.055	1.5680 ²⁰		262–264	>112	
d456	2,6-Dimethoxy- pyridine	$(CH_3O)_2C_5H_3N$	139.15		1.053	1.5029^{20}		178–180	61	
d457	2,5-Dimethoxytetra- hydrofuran	(CH ₃ O) ₂ C ₄ H ₆ O	132.16		1.020	1.4180^{20}		145–147	35	
d458	<i>N,N</i> -Dimethylacetamide	CH ₃ C(O)N(CH ₃) ₂	87.12	4, 59	0.9366 ²⁵	1.4356 ²⁵	-20	165.5	70	misc aq, alc, bz, eth
d459	Dimethyl 1,3- acetone- dicarboxylate	[CH ₃ OOCCH ₂] ₂ C=O	174.15	3,790	1.185	1.4434 ²⁰		150 ^{25mm}	>112	
d460	Dimethyl acetylene- dicarboxylate	CH₃OOCC≡CCOOCH₃	142.11	2, 803	1.156	1.4470^{20}		95-98 ^{19mm}	86	
d461	Dimethylamine	(CH ₃) ₂ NH	45.09	4, 39	0.680_4^0		-92.2	6.9		v s aq; s alc, eth

Dimethyl acetal, d438 Dimethylacetic acid, m390 2,3-Dimethylacrylic acids, m161, m162

3,3-Dimethylacrylic acid, m163

3,3-Dimethylallene, m148 Dimethylaminoacetaldehyde diethyl acetal, d249

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d462	4-Dimethylamino-	(CH ₃) ₂ NC ₆ H ₄ CHO	149.19	14, 31			74	176 ^{17mm}		s alc, chl, eth,
d463	benzaldehyde p-(Dimethylamino)- benzenesulfonic	(CH ₃) ₂ NC ₆ H ₄ SO ₃ ⁻ Na ⁺	223.23	14 ³ , 2023			>300			НОАс
d464	acid, Na salt 4-Dimethylamino- benzoic acid	(CH ₃) ₂ NC ₆ H ₄ COOH	165.19	14, 426			241 d			s alc; sl s eth
d465	2-(Dimethylamino)- ethanol	(CH ₃) ₂ NCH ₂ CH ₂ OH	89.14	4, 276	0.8876_4^{20}	1.4294 ²⁰		135	40	misc aq, alc, eth
d466	2-(Dimethylamino)- ethyl benzoate	C ₆ H ₅ COOCH ₂ CH ₂ - N(CH ₃) ₂	193.26		1.014	1.5077 ²⁰		155 ^{20mm}		
d467	2-Dimethylamino- ethyl chloride HCl	(CH ₃) ₂ NCH ₂ CH ₂ Cl·HCl	144.05	4, 133			205–208			
d468	2-(Dimethylamino)- ethyl methacrylate	H ₂ C=C(CH ₃)COOCH ₂ - CH ₃ N(CH ₃) ₂	157.22	4 ³ , 649	0.933	1.439120		182–192	70	
d469	4-Dimethylamino-3- methyl-2-butanone	(CH ₃) ₂ NCH ₂ CH(CH ₃)- COCH ₃	129.20	41, 452	0.841	1.4250 ²⁰		73 ^{35mm}	38	
d470	3-Dimethylamino- phenol	(CH ₃) ₂ NC ₆ H ₄ OH	137.18	13, 405	1.5895 ²⁶		82–84	265–268		v s alc, bz, eth, acet
d471	3-(Dimethylamino)- 1,2-propanediol	(CH ₃) ₂ NCH ₂ CH(OH)- CH ₂ OH	119.16	4, 302	1.004	1.4609 ²⁰		216–217	105	s aq, alc, chl, eth
d472	1-Dimethylamino-2- propanol	CH ₃ CH(OH)CH ₂ N(CH ₃) ₂	103.17		0.837	1.419320		121–127	35	
d473	3-Dimethylamino-1- propanol	(CH ₃) ₂ NCH ₂ CH ₂ CH ₂ OH	103.17	4 ¹ , 433	0.872	1.4360 ²⁰		163–164	36	
d474	3-(Dimethylamino)- propionitrile	(CH ₃) ₂ NCH ₂ CH ₂ CN	98.15	4 ³ , 1265	0.870	1.4258 ²⁰	-43	171 ^{750mm}	62	
d475	3-Dimethyl- aminopropyl chloride HCl	(CH ₃) ₂ NCH ₂ CH ₂ - CH ₂ Cl·HCl	158.07	4, 148			141–144		35	

d476	4-(Dimethylamino)-	$(CH_3)_2N(C_5H_4N)$	122.17	222, 341			108-110			v s aq, alc, bz, chl
d477	pyridine N,N-Dimethyl-	C ₆ H ₅ N(CH ₃) ₂	121.18	12, 141	0.9559_4^{20}	1.5584 ²⁰	2.5	194.2	62	v s alc, chl, eth
d478	aniline 2,3-Dimethyl- aniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1101	0.993120	1.5685 ²⁰	2.5	221–222	96	sl s aq; s alc, eth
d479	2,4-Dimethyl-	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1111	0.980_4^{20}	1.5586^{20}		218	90	s alc, bz, eth
d480	2,5-Dimethyl- aniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1135	0.9790_4^{21}	1.559220	11.5	218	93	sl s aq; s alc, eth
d481	2,6-Dimethyl- aniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1107	0.984 ²⁰	1.5601 ²⁰	10–12	216	91	sl s aq; s alc, eth
d482	3,4-Dimethylaniline	$(CH_3)_2C_6H_3NH_2$	121.18	12, 1103	1.07618	4 5 5 5 0 20	49–51	226		sl s aq; s alc
d483 d484	3,5-Dimethylaniline Dimethylarsinic acid	(CH ₃) ₂ C ₆ H ₃ NH ₂ (CH ₃) ₂ As(O)OH	121.18 137.99	12, 1131	0.972_4^{20}	1.5578 ²⁰	195–196	104 ^{14mm}	93	sl s aq; s alc v s alc; 200 aq; i eth
d485	3,4-Dimethylbenzoic acid	$(CH_3)_2C_6H_3COOH$	150.18	$9^2,353$			165–167	subl		s alc, bz
d486	2,5-Dimethylbenzo- nitrile	$(CH_3)_2C_6H_3CN$	131.18	9, 535	0.957	1.5284 ²⁰	13–14	223 ^{730mm}	92	
d487	N,N-Dimethylbenzyl- amine	$C_6H_5CH_2N(CH_3)_2$	135.21	12, 1019	0.900	1.5011 ²⁰	-75	183	54	
d488	2,3-Dimethyl-1,3- butadiene	$H_2C = C(CH_3)C$ - $(CH_3) = CH_2$	82.15	1 ³ , 991	0.7222_4^{25}	1.4362 ²⁵	-76.0	69.2	<1	
d489	2,2-Dimethylbutane	CH ₃ CH ₂ C(CH ₃) ₃	86.18	1, 150	0.6492^{20}	1.3688^{20}	-99.9	49.7	-28	
d490	2,3-Dimethylbutane	(CH ₃) ₂ CHCH(CH ₃) ₂	86.18	1, 151	0.6616^{20}	1.3750^{20}	-128.5	58.0	-28	
d491	2,3-Dimethyl-2-3-	$(CH_3)_2C(OH)C(OH)$ -	118.18	1,487			41.1	174.4		v s hot aq, alc, eth
	butanediol	$(CH_3)_2$								

3-Dimethylaminopropylamine, d593 Dimethylanisoles, d547, d548 2,4-Dimethyl-3-azapentane, d411 Dimethylbenzenes, x4, x5, x6 6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol, n105 Dimethyl (Z)-butenedioate, d544

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d492	2,2-Dimethyl-1-	CH ₃ CH ₂ C(CH ₃) ₂ CH ₂ OH	102.18	1 ³ , 1675	0.8286420	1.420820	<-15	136.8		sl s aq; s alc, eth
d493	2,3-Dimethyl-1- butanol	(CH ₃) ₂ CHCH(CH ₃)- CH ₂ OH	102.18	1 ³ , 1677	0.8300_4^{20}	1.4205 ²⁰		149		s alc, eth
d494	2,3-Dimethyl-2- butanol	(CH ₃) ₂ CHC(CH ₃) ₂ OH	102.18	1,413	0.8236_4^{20}	1.4176 ²⁰	-10.6	118.7	29	s aq; misc alc, eth
d495	3,3-Dimethyl-1- butanol	(CH ₃) ₃ CCH ₂ CH ₂ OH	102.18	1 ³ , 1677	0.8147 ²⁰	1.4120^{20}	-60	143	47	s alc, eth
d496	3,3-Dimethyl-2- butanol	(CH ₃) ₃ CCH(OH)CH ₃	102.18	1,412	0.8185_4^{20}	1.4151 ²⁰	5.3	120.4	28	s alc; misc eth
d497	3,3-Dimethyl-2- butanone	(CH ₃) ₃ CCOCH ₃	100.16	1,694	0.7250_{25}^{25}	1.3939 ²⁵	-52.5	106.2	23	2.5 aq; s alc, eth
d498	2,3-Dimethyl-2- butene	$(CH_3)_2C = C(CH_3)_2$	84.16	1, 218	0.7081_4^{20}	1.4124 ²⁰	-74.3	73.2	-16	s alc, eth
d499	3,3-Dimethyl-1- butene	(CH ₃) ₃ CCH=CH ₂	84.16	1, 217	0.6531_4^{20}	1.376220	-115.2	41.3	-28	
d500	3,3-Dimethylbutyric acid	(CH ₃) ₃ CCH ₂ COOH	116.16	2, 337	0.9124_4^{20}	1.4100^{20}	6–7	190	88	s alc, eth
d501	Dimethylcadmium	(CH ₃) ₂ Cd	142.48		1.984647	1.5488	-4.5	105.5	≥150 ex-	d aq; s PE
									plo- des	
d502	Dimethylcarbamyl chloride	(CH ₃) ₂ NCOCl	107.54	4, 73	1.168	1.4540^{20}	-33	168	68	
d503 d504	Dimethyl carbonate Dimethyl chlorothio-	(CH ₃ O) ₂ C=O (CH ₃ O) ₂ P(S)Cl	90.08 160.56	3, 4 1 ¹ , 143	1.065 ¹⁷ 1.322	$1.3682^{20} \\ 1.4819^{20}$	0.5	90–91 67 ^{16mm}	18	i aq; misc alc, eth
	phosphate	, , , , ,						0,		
d505	Dimethylcyanamide	$(CH_3)_2NCN$	70.09	4, 74	0.867	1.4100^{20}		161–163	58	

d506	cis-1,2-Dimethyl-cyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 36	0.7692_4^{20}	1.4335 ²⁰	-49.9	129.7	15	i aq; s alc, bz
d507	trans-1,2-Dimethyl- cyclohexane	$(CH_3)_2C_6H_{10}$	112.22	5, 36	0.7772_0^{20}	1.4273 ²⁰	-88.2	123.4	15	i aq; s alc, eth
d508	5,5-Dimethyl-1,3- cyclohexanedione		140.18	7, 559			d 149			0.4 aq; s alc, bz
d509	2,3-Dimethylcyclo- hexanol	$(CH_3)_2C_6H_9OH$	128.22		0.934	1.4653 ²⁰			65	
d510	2,6-Dimethylcyclo- hexanone		126.20	7, 23	0.925	1.4460 ²⁰		175	51	i aq; s alc, eth
d511	2,3-Dimethylcyclo- hexylamine	$(CH_3)_2C_6H_9NH_2$	127.23		0.835	1.4595 ²⁰		160	51	
d512	Dimethyl decanedioate	CH ₃ OOC(CH ₂) ₈ COOCH ₃	230.30	2,719	0.983_{20}^{30}	1.4335 ²⁸	23	144 ^{5mm}		i aq; s alc, eth
d513	5,7-Dimethyl-3,5,9- decatrien-2-one	H ₂ C=CHCH ₂ CH(CH ₃)- CH=C(CH ₃)CH=CH- COCH ₃	178.28					79 ^{0.05mm}		
d514	Dimethyl 2,5-dioxo- 1,4-cyclohexanedi- carboxylate		228.20	10, 894			155–157			

Dimethyl 2-butynedioate, d460 Dimethyl Cellosolve, d439 Dimethylchlorosilane, c92 (Z)-2-Dimethylcrotonic acid, m162 Dimethyl 1,4-cyclohexanedione-2,5dicarboxylic acid, d514 Dimethyl diphenyl sulfone 4,4'-dicarboxylate, s26

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d515	2,3-Dimethyl-1,3- dioxolane-4- methanol		132.16		1.064 ²⁰	1.4383 ²⁰		188–189	80	misc aq, alc, eth
d516 d517	Dimethyl disulfide Dimethyldithio- carbamic acid dihydrate, Na salt	$\begin{array}{c} CH_3SSCH_3\\ (CH_3)_2NCSS^-Na^+ \cdot \\ 2H_2O \end{array}$	94.20 179.24	1, 291 4, 75	1.046	1.5253 ²⁰	-84.7	109.8	24	i aq; misc alc, eth
d518	Dimethyl ether	(CH ₃) ₂ O	46.07	1, 281	0.661 ²⁰		-141.5	-24.9	-41	35% aq (5 atm); 15% bz; 11.8% acet
d519	Dimethylethoxy- phenylsilane	$C_2H_5O(C_6H_5)Si(CH_3)_2$	180.3		0.9263_4^{20}	1.4799^{20}		93 ^{35mm}		
d520	N,N-Dimethylethyl- amine	$C_2H_5N(CH_3)_2$	73.14	4, 94	0.675	1.3720^{20}	-140	36–38	-36	
d521	N,N-Dimethylethyl- enediamine	(CH ₃) ₂ NCH ₂ CH ₂ NH ₂	88.15	$4^2,690$	0.803	1.4260^{20}			23	
d522	N,N-Dimethyl- formamide	(CH ₃) ₂ NCHO	73.10	4, 58	0.9445_4^{25}	1.4282 ²⁵	-60.4	153.0	57	misc aq, alc, bz, eth
d523	N,N-Dimethyl- formamide dimethyl acetal	(CH ₃) ₂ NCH(OCH ₃) ₂	119.16		0.897	1.3972 ²⁰		103 ^{720mm}	7	
d524	Dimethyl fumarate	CH ₃ OOCCH=CHCOOCH ₃	144.13	2, 741	1.045^{106}		105	193		sl s alc, eth
d525	2,5-Dimethylfuran	$(CH_3)_2(C_4H_2O)$	96.13	17, 41	0.9000_4^{20}	1.4414^{20}	-62	93	<1	i aq; misc alc, eth
d526	Dimethylglyoxime	$CH_3C(=NOH)C-$ $(=NOH)CH_3$	116.12	1,772			238–240			s alc, acet, eth, pyr
d527	2,4-Dimethyl-2,6- heptadienal	H ₂ C=CHCH ₂ CH(CH ₃)- CH=C(CH ₃)CHO	138.21					47 ^{2mm}		
d528	2,4-Dimethyl-2,6- heptadien-1-ol	H ₂ C=CHCH ₂ CH(CH ₃)- CH=C(CH ₃)CH ₂ OH	140.23					88 ^{10mm}		

d529	2,6-Dimethyl-2,5-	$(CH_3)_2C = CHC (= 0)$ -	138.21	1,751	0.885_4^{20}	1.4968^{21}	28	198–199	79	sl s aq; s alc, eth
	heptadien-4-one	$CH = C(CH_3)_2$								
d530	Dimethyl	CH ₃ OOC(CH ₂) ₅ COOCH ₃	188.22	2 ¹ , 281	1.0625_4^{20}	1.4314^{20}	-21	122 ^{11mm}	>112	s alc
	heptanedioate									
d531	2,6-Dimethyl-4-	$[(CH_3)_2CHCH_2]_2C=O$	142.24	1,710	0.806_{20}^{20}	1.4114^{20}	-41.5	168.1	48	0.06 aq; misc alc,
	heptanone									bz, chl, eth
d532	2,5-Dimethyl-2,4-	$(CH_3)_2C$ = $CHCH$ = C -	110.20	1, 259	0.7636_4^{20}	1.4741^{20}	12-14	132–134	29	i aq; s alc, eth
	hexadiene	$(CH_3)_2$								
d533	2,5-Dimethylhexane	(CH ₃) ₂ CHCH ₂ CH ₂ -	114.24	$1^3, 283$	0.6936_4^{20}	1.3925^{20}	-91.2	109.1	26	i aq; sl s alc; s eth
		CH(CH ₃) ₂								
d534	2,5-Dimethyl-2,5-	[(CH3)2C(NH2)CH2]2	144.26		0.832	1.4459^{20}		64 ^{8mm}	62	
	hexanediamine									
d534a	Dimethyl	CH ₃ OOC(CH ₂) ₄ COOCH ₃	174.20	1,652	1.0600_4^{20}	1.4285^{20}	8	112 ^{10mm}	107	i aq; s alc, eth
	hexanedioate									
d535	2,5-Dimethyl-2,5-	$[(CH_3)_2C(OH)CH_2-]_2$	146.23	1,492			86-90	214-215	126	
	hexanediol									
d536	1,5-Dimethylhexyl-	(CH ₃) ₂ CH(CH ₂) ₃ -	129.25		0.767	1.4209^{20}		154-156	48	
	amine	CH(NH ₂)CH ₃								
d537	2,5-Dimethyl-3-	$(CH_3)_2CC \equiv CC(CH_3)_2$	142.20	1,501			94–95	205-206		
	hexyne-2,5-diol	ОНОН								
	1	'		'	1		1	1		'

Dimethyleneimine, e131 Dimethylene oxide, e129 *N,N*-Dimethylethanolamine, d465 Dimethyl glutarate, d574 Dimethylglutaric acids, d575, d576

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d538	5,5-Dimethyl- hydantoin		128.13	24, 289			176–178			v s aq, alc, bz, chl, eth, acet
d539	1,1-Dimethyl- hydrazine	(CH ₃) ₂ NNH ₂	60.10	4, 547	0.791422	1.4075 ²⁰	-58	63.9	1	misc aq, alc, eth, PE
d540	1,2-Dimethyl- hydrazine	CH ₃ NHNHCH ₃	60.10	4, 547	0.8274_4^{20}	1.4209 ²⁰		81	flamm- able	misc aq, alc, eth, PE
d541	Dimethyl hydrogen phosphonate	$(CH_3O)_2P(=O)H$	110.05	1, 285	1.200_4^{20}	1.4009 ²⁰		170–171	96	s aq(hyd); misc alc, acet, eth
d542	1,2-Dimethyl- imidazole		96.13	23, 66	1.084		29–30	204	92	
d543	1,3-Dimethyl-2- imidazolidinone		114.15		1.044	1.4720 ²⁰		108 ^{17mm}	80	
d543a	Dimethylketene	$(CH_3)_2C=C=O$	70.09	1,731			-97.5	34		d aq, alc; s eth
d544	Dimethyl maleate	CH ₃ OOCCH=CHCOOCH ₃	144.13	2, 751	1.1513^{20}	1.4422^{20}	-17.5	200.4		8.7 aq
d545	Dimethyl malonate	CH ₃ OOCCH ₂ COOCH ₃	132.12	2, 572	1.154_4^{20}	1.4135 ²⁰	-62	180–181	90	sl s aq; misc alc, eth
d546	Dimethylmercury	$(CH_3)_2Hg$	230.66	4, 678	3.1874^{20}	1.5452^{20}		92 ^{740mm}		i aq; s alc, eth
d547	3,4-Dimethyl-1- methoxybenzene	$(CH_3)_2C_6H_3OCH_3$	136.19	6, 481	0.9744_4^{14}	1.519814		200		i aq; s alc, bz, eth
d548	3,5-Dimethyl-1- methoxybenzene	$(CH_3)_2C_6H_3OCH_3$	136.19	6, 493	0.962745	1.510715		193	65	i aq; s alc, bz, eth
d549	N,N-Dimethylmethyl- eneammonium iodide	$H_2C = N(CH_3)_2^+I^-$	185.01	4 ⁴ , 153			219 d			
d550	Dimethyl methylene- succinate	CH ₃ OOCCH ₂ C(=CH ₂)- COOCH ₃	158.15	2,762	1.124148	1.4442 ²⁰	38	208		s alc, eth
d551	Dimethyl methyl- phosphonate	(CH ₃ O) ₂ P(O)CH ₃	124.08	4 ¹ , 572	1.145	1.4130 ²⁰		181	43	
d552	Dimethyl methyl- succinate	CH ₃ OOCCH ₂ CH(CH ₃)- COOCH ₃	160.17	2 ³ , 1696	1.076	1.4200 ²⁰		196	83	

d553	2,6-Dimethyl-		115.18		0.9346 ²⁰	1.4470^{20}	-85	147	48	misc aq, alc, bz
d554	morpholine 2,3-Dimethyl- naphthalene	$(CH_3)_2C_{10}H_6$	156.23	5, 571	1.00820		102–104	269		sl s alc; s bz, eth
d555	2,6-Dimethyl- naphthalene	$(CH_3)_2C_{10}H_6$	156.23	5, 570	1.1424		110.2	262		i aq; sl s alc
d556	1,2-Dimethyl-3- nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 367	1.129	1.5434 ²⁰	7–9	245	107	i aq; s alc
d557	1,2-Dimethyl-4- nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 368	1.139		29–31	143 ^{20mm}		i aq; s alc
d558	1,3-Dimethyl-2- nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 378	1.112	1.5220^{20}	14–16	225 ^{744mm}	87	i aq; s alc
d559	1,3-Dimethyl-4- nitrobenzene	$(CH_3)_2C_6H_3NO_2$	151.17	5, 378	1.117	1.5497 ²⁰	2	237–239	107	s alc, bz, chl, eth
d560	N,N-Dimethyl-4- nitrosoaniline	(CH ₃) ₂ NC ₆ H ₄ NO	150.18	12,677			86	flammable solid		i aq; s alc, eth
d561	Dimethyl 2-nitro- 1,4-phthalate	O ₂ NC ₆ H ₃ (COOCH ₃) ₂	239.18	9, 826			72–75			

Dimethyl isophthalate, d589 1,4*a*-Dimethyl-7-isopropyl-1,2,3,4,4*a*,9,10,10*a*-octahydro-1-phenanthrenemethylamine, d20 Dimethyl itaconate, d550 2,2-Dimethyl-3-methylenenorbornane, c2 6,6-Dimethyl-2-methylenenorpinene, p176

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d562	cis-3,7-Dimethyl-		152.24		0.8888_4^{20}	1.489820		229	101	misc alc, eth, glyc
d563	2,6-octadienal trans-3,7-Dimethyl-2,6-octadienal		152.24		0.8869_4^{20}	1.4869 ²⁰		229	101	misc alc, eth, glyc
d564	3,7-Dimethyl-2,6- octadienenitrile		149.24		0.853	1.4753 ²⁰			>112	
d565	Dimethyl octanedioate	CH ₃ OOC(CH ₂) ₆ COOCH ₃	202.25	2, 693	1.0210_4^{20}	1.432520	-4.8	268		i aq; s alc
d566	Dimethyl oxalate	CH ₃ OOCCOOCH ₃	118.08	2, 534	1.14854	1.37980	50–54	163.5	75	6 aq; s alc, eth
d567	N¹-(4,5-Dimethyl- oxazol-2-yl)- sulfanilamide		267.31				193–194			s aq, acids, alk
d568	N-(1,1-Dimethyl-3-oxobutyl)acryl-amide	CH ₂ =CHC(=O)NHC- (CH ₃) ₂ CH ₂ COCH ₃	169.23				57–58	120 ^{8mm}		
d569	2,3-Dimethylpentanal	CH ₃ CH ₂ CH(CH ₃)CH- (CH ₃)CHO	114.19		0.832	1.413220			58	
d570	2,2-Dimethylpentane	CH ₃ CH ₂ CH ₂ C(CH ₃) ₃	100.21	1, 157	0.674_4^{20}	1.382420	-123.8	79.2	15	i aq; s alc, eth
d571	2,3-Dimethylpentane	CH ₃ CH ₂ CH(CH ₃)- CH(CH ₃) ₂	100.21	1^2 , 120	0.6951_4^{20}	1.3920 ²⁰	glass	89.8	-6	i aq; s alc, eth
d572	2,4-Dimethylpentane	(CH ₃) ₂ CHCH ₂ CH(CH ₃) ₂	100.21		0.6727_4^{20}	1.3815^{20}	-119.2	80.5		s alc, eth
d573	3,3-Dimethylpentane	CH ₃ CH ₂ C(CH ₃) ₂ CH ₂ CH ₃	100.21	1, 158	0.6933_4^{20}	1.3905^{20}	-134.4	86.1	-6	i aq; s alc, eth
d574	Dimethyl pentanedioate	CH ₃ OOC(CH ₂) ₃ - COOCH ₃	160.17	2, 633	1.093445	1.4234 ²⁰		94–95 ^{13mm}	102	v s alc, eth
d575	2,2-Dimethyl- pentanedioic acid	HOOCC(CH ₃) ₂ CH ₂ - CH ₂ COOH	160.17	2, 676			83–85			v s aq, alc, chl
d576	3,3-Dimethyl- pentanedioic acid	(CH ₃) ₂ C(CH ₂ COOH) ₂	160.17	2, 684			100–103			v s aq, alc, eth

d577	2,4-Dimethyl-3-	(CH ₃) ₂ CHCH(OH)-	116.20	1,417	0.829_4^{20}	1.4254^{20}	< 70	140	37	sl s aq; s alc, eth
	pentanol	CH(CH ₃) ₂								
d578	2,4-Dimethyl-3-	$(CH_3)_2CHC(=O)$ -	114.19	1,703	0.8062_4^{20}	1.3986^{20}	-80	124	15	misc alc, eth; s bz
	pentanone	CH(CH ₃) ₂								
d579	2,3-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 480		1.5420^{20}	75	218		v s alc, bz, chl, eth
d580	2,4-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 486	1.0276_4^{14}	1.5390^{20}	27	210-212	>112	v s alc, bz, chl, eth
d581	2,5-Dimethylphenol	(CH ₃) ₂ C ₆ H ₃ OH	122.17	6, 494	0.965^{80}		74.5	211.5		v s alc, bz, chl, eth
d582	2,6-Dimethylphenol	(CH ₃) ₂ C ₆ H ₃ OH	122.17	6, 485			49.0	203	73	v s alc, bz, chl, eth
d583	3,4-Dimethylphenol	$(CH_3)_2C_6H_3OH$	122.17	6, 480	1.064_4^{28}		62.5	225		v s alc, bz, chl, eth
d584	3,5-Dimethylphenol	(CH ₃) ₂ C ₆ H ₃ OH	122.17	6, 492	1.008_4^{28}		64-68	219.5		v s alc, bz, chl, eth
d585	Dimethylphenyl-	(CH ₃) ₂ Si(Cl)C ₆ H ₅	170.7		1.032_4^{20}	1.508^{20}		192-193		
	chlorosilane									
d586	4,5-Dimethyl-o-	$(CH_3)_2C_6H_2(NH_2)_2$	136.20	13, 179			127-129			
	phenylenediamine									
d587	Dimethylphenyl-	(CH ₃) ₂ Si(H)C ₆ H ₅	136.3		0.8891_4^{20}	1.4995^{20}		156-157		
	silane									
	I	1	1	I	1		I	l		

3,7-Dimethyl-6-octen-1-o1, c274 Dimethylolpropionic acid,

Dimethyl 3-oxoglutarate, d459 2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one, a309 1,5-Dimethyl-2-phenyl-4-aminopyrazolone, a113

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d588	Dimethyl-o-	C ₆ H ₄ (COOCH ₃) ₂	194.19	9, 797	1.1940^{20}_{20}	1.515 ²¹	5.5	283.7	146	0.4 aq; misc alc,
d589	phthalate Dimethyl- <i>m</i> - phthalate	C ₆ H ₄ (COOCH ₃) ₂	194.19	9, 834	1.194_4^{20}	1.5168 ²⁰	67–68	282		chl, eth; i PE i aq
d590	Dimethyl -p- phthalate	C ₆ H ₄ (COOCH ₃) ₂	194.19	4.3303	1.2		140–142	288		i aq, hot alc,eth
d591	2,6-Dimethyl- piperidine		113.20	20, 108	0.840	1.439420		127	11	
d592 d593	2,2-Dimethylpropane <i>N,N</i> -Dimethyl-1,3-	(CH ₃) ₄ C (CH ₃) ₂ N(CH ₂) ₃ NH ₂	72.15 102.18		0.613 ⁰ 0.812	1.3476^6 1.4350^{20}	-16.6	9.5 123	35	
u393	propanediamine	(C113)214(C112)314112	102.16			1.4330		123	33	
d594	2,2-Dimethyl-1,3- propanediol	$(CH_3)_2C(CH_2OH)_2$	104.15	1, 483	1.11 ²⁵		127–128	208–210		180 aq; 12 bz; 60 acet; v s alc, eth
d595	2,2-Dimethyl-1- propanol	(CH ₃) ₃ CCH ₂ OH	88.15	1,406	0.812_4^{20}		52–54	113.1	36	3.6 aq; misc alc, eth
d596	2,2-Dimethylpropion- aldehyde	(CH ₃) ₃ CCHO	186.25		0.793	1.3794 ²⁰	6	74 ^{730mm}	<1	
d597	2,2-Dimethyl propionamide	(CH ₃) ₃ CC(O)NH ₂	101.15	2, 320			154–157	212		
d598	2,2-Dimethyl- propionic acid	(CH ₃) ₃ CCOOH	102.13	2, 319	0.90550	1.3931 ³⁷	35.5	163.8	63	2.5 aq; v s alc, eth
d599	2,2-Dimethylpro-	[(CH ₃) ₃ CC(O)] ₂ O	186.25	2, 320	0.918	1.4092^{20}		193	57	
d600	2,2-Dimethyl- propionyl chloride	(CH ₃) ₃ CCOCl	120.58	2, 320	0.979	1.4120^{20}		105–106	<1	d aq, alc; v s eth
d601	1,1-Dimethyl- propylamine	CH ₃ CH ₂ C(CH ₃) ₂ NH ₂	87.17	4, 179	0.731_4^{25}	1.3996^{20}	-105	77	65	misc aq, alc, eth
d602	1,1-Dimethyl-2- propynylamine	HC≡CC(CH ₃) ₂ NH ₂	83.13		0.790	1.4235 ²⁰		79–80	<1	

d603	3,5-Dimethyl-		96.13	23,74			108	218	I	s aq; v s bz, eth
	pyrazole		, , , , ,	_==,						
d604	2,4-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 244	0.927_4^{25}	1.4991^{20}	<-60	158.3	37	17 aq; v s alc, bz,
										eth
d605	2,6-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 244	0.9200_4^{25}	1.4956^{25}	-6.0	143-144	33	43 aq ⁴⁵ ; s alc, eth
d606	3,4-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 246	0.939_4^{25}	1.5100^{25}	-12	164	53	sl s aq; s alc, eth
d607	3,5-Dimethylpyridine	$(CH_3)_2(C_5H_3N)$	107.16	20, 246	0.939_4^{25}	1.5033^{25}	-9	170	53	s aq, alc, eth
d608	Dimethyl succinate	CH ₃ OOCCH ₂ CH ₂ COOCH ₃	146.14	2,609	1.202_4^{18}	1.4190^{20}	19.5	195-200	85	0.83 aq; 2.9 alc
d609	Dimethylsulfamoyl	(CH ₃) ₂ NSO ₂ Cl	143.59	4, 84	1.337	1.4518^{20}		114 ^{75mm}		
	chloride									
d610	Dimethyl sulfate	$(CH_3O)_2SO_2$	126.13	1, 283	1.3322_4^{20}	1.3874^{20}	-31.8	188 d	83	2.8 aq(hyd); s
										acet, bz, diox,
										eth
d611	Dimethyl sulfide	$(CH_3)_2S$	62.13	1, 288	0.846_4^{21}	1.4354^{20}	-98.3	37.3	-36	2 aq; s alc, eth
d612	Dimethyl sulfite	(CH ₃ O) ₂ SO	110.13	1, 282	1.294	1.4083^{20}		126–127	30	
d613	Dimethyl sulfone	$(CH_3)_2SO_2$	94.13	1, 289			109	238	143	v s aq, alc, acet
d614	Dimethyl sulfoxide	(CH ₃) ₂ SO	78.13	1, 289	1.100_4^{20}	1.4783^{20}	18.5	189.0	95	s alc, acet, bz, chl
d615	Dimethyl- d_6	(CD ₃) ₂ SO	84.18		1.18	1.4758^{20}		55 ^{5mm}	95	
	sulfoxide									

Dimethyl phosphite, d541 Dimethyl pimelate, d530 Dimethyl propanedioate, d545 1,1-Dimethylpropargylamine, d602 N'-(4,6-Dimethyl-2-pyrimidinyl)sulfanilamide, s21

Dimethyl sebacate, d512 Dimethyl suberate, d565

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d616	(+)-Dimethyl- L-tartrate	CH ₃ OOCCH(OH)CH(OH)- COOCH ₃	178.14	3,510	1.328420		48-50	163 ^{23mm}		s aq; 200 alc ¹⁵ ; v s bz
d617	Dimethyltelluride	(CH ₃) ₂ Te	157.68	1, 291			-10	91–92		d aq; v s alc; i eth
d618	2,5-Dimethyltetra-	$(CH_3)_2 Ie$ $(CH_3)_2 (C_4 H_6 O)$	100.16	17, 14	0.833	1.4041	-10	90–92	26	d aq, v s alc, i etti
uoro	hydrofuran	$(C11_3)_2(C_411_6O)$	100.10	17,14	0.833	1.4041		90-92	20	
d619	Dimethyl-3,3'-	(CH ₃ OOCCH ₂ CH ₂) ₂ S	206.26		1.198	1.4740 ²⁰		148 ^{18mm}	>112	
d620	thiodipropionate N,N-Dimethylthio-	(CIL) NC(S)II	89.16	4, 70	1.047	1.5757 ²⁰		58 ^{1mm}	99	
0020	formamide	(CH ₃) ₂ NC(S)H	89.10	4, 70	1.047	1.3/3/		36	99	
d621	<i>N,N'</i> -Dimethylthio-	(CH ₂ NH) ₂ C=S	104.18	4,70			60–62			v s aq, alc, acet
0021	urea	(CH31111)2C—5	104.10	7, 70			00 02			v s aq, arc, acct
d622	N,N-Dimethyl-p-	$CH_3C_6H_4N(CH_3)_2$	135.21	12,902	0.937	1.5458 ²⁰		211	83	
d623	1,3-Dimethylurea	(CH ₃ NH) ₂ C=O	88.11	4, 65			101-104	268-270		v s ag, alc, i eth
d624	Dimethylzinc	(CH ₃) ₂ Zn	95.45	,	1.386411		-40	46	ignites	misc bz, PE; s eth
	•								in air	
d625	2,4-Dinitroaniline	$(O_2N)_2C_6H_3NH_2$	183.12	12, 747	1.615^{14}		188			i aq; 0.75 alc
d626	1,3-Dinitrobenzene	$C_6H_4(NO_2)_2$	168.11	5, 258	1.575_4^{18}		89–90	300-303		0.05 aq; 2.7 alc; v
										s bz, chl, EtAc
d627	2,4-Dinitrobenzene-	$(O_2N)_2C_6H_3SC1$	234.62	$6^2,316$			96			s bz, HOAc; d alc
	sulfenyl chloride									
d628	3,4-Dinitrobenzoic acid	$(O_2N)_2C_6H_3COOH$	212.12	9,413			166	subl		0.7 aq; v s alc, eth
d629	3,5-Dinitrobenzoic	$(O_2N)_2C_6H_3COOH$	212.12	9,413			207			1.9 hot aq; v s alc;
d630	acid	(O N) C H COCI	220.56	9, 414			69.5	196 ^{11mm}		sl s bz, eth
0030	3,5-Dinitrobenzoyl chloride	(O ₂ N) ₂ C ₆ H ₃ COCl	230.56	9,414			09.3	190		d aq, alc; s eth
d631	2,6-Dinitro-p-cresol	$(O_2N)_2C_6H_2(OH)CH_3$	198.13	6, 414			77–79			
	_						(an-			
							hyd)			

d631a	4,6-Dinitro-o-cresol	$(O_2N)_2C_6H_2(OH)CH_3$	198.13	6, 368			87.5			v s alc, acet, eth,
d632	1.1-Dinitroethane	CH ₃ CH(NO ₂) ₂	120.07	1, 102	1.350324			185–186		s alc, eth
d633	2.4-Dinitro-1-	1 3 1 2/2	186.10	l '	1.5505 ₂₄	1.5690^{20}	26	178 ^{25mm}	>112	· '
0033	fluorobenzene	$FC_6H_3(NO_2)_2$	180.10	5, 262		1.3090	20	1/6	<i>></i> 112	s bz, eth, glyc
d634	1,5-Dinitro- naphthalene	$C_{10}H_6(NO_2)_2$	218.17	5, 558			216–217	subl		s bz; v s eth; sl s
d635	2,4-Dinitrophenol	$(O_2N)_2C_6H_3OH$	184.11	6, 251	1.683		112-114			s alc, bz; 16 EtAc;
										36 acet; 5 chl;
										20 pyr
d636	2,4-Dinitrophenyl-	$(O_2N)_2C_6H_3CH_2COOH$	226.15	9, 459			169–175			s alc, eth
	acetic acid									
d637	2,4-Dinitrophenyl-	$(O_2N)_2C_6H_3NHNH_2$	198.14	15, 489			~200	flammable		sl s aq, alc; s acid
	hydrazine							solid		
d638	3,5-Dinitrosalicyclic	$(O_2N)_2C_6H_2(OH)COOH$	228.12	10, 122			169–172			s aq; v s alc, eth
	acid									
d639	2,4-Dinitrotoluene	$CH_3C_6H_3(NO_2)_2$	182.14	5, 339	1.32171	1.442	64.66	300 sl d		1.2 alc; 9 eth
d640	2,6-Dinitrotoluene	$CH_3C_6H_3(NO_2)_2$	182.14	5, 341	1.2833111	1.479	64–66			s alc
d641	3,4-Dinitrotoluene	$CH_3C_6H_3(NO_2)_2$	182.14	5, 341	1.2594111		54-57			i aq; s alc
d641a	Dinonyl hexanedioate	$C_9H_{19}OOC(CH_2)_4$ -	398.63		0.917^{25}_{25}				218	
		COOC ₉ H ₁₉								
d642	Dioctadecyl	$(C_{18}H_{37}O)P(O)H$	586.97				57-59			
	phosphite									
d643	Dioctylamine	$(C_8H_{17})_2NH$	241.46	4, 196			14-16	298	>112	i aq; v s alc, eth
d644	Dioctyl sulfide	$(C_8H_{17})_2S$	258.51	1,419	0.842	1.4610^{20}		180 ^{10mm}	>112	
d645	4,9-Dioxa-1,12-	H ₂ N(CH ₂) ₃ O(CH ₂) ₄ -	204.32		0.962	1.4609^{20}		134-	>112	
	dodecanediamine	O(CH ₂) ₃ NH ₂						136 ^{4mm}		
	1	I	l	l	1 1					I

Dimethyl terephthalate, d590 2,3-Dimethylvaleraldehyde, d569 2,4-Dinitrochlorobenzene, c94 3,4-Dinitrochlorobenzene, c95 3,5-Dinitro-1-toluic acid, m228 Dioctyl phthalates, b179, d313 6,8-Dioxabicylco[3.2.1]octan-7-one, h183

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d646	1,4-Dioxane		88.10	19, 3	1.0329_4^{20}	1.4224 ²⁰	11.7	101.2	12	misc aq, alc, bz, chl, eth, PE
d647 d648	1,3-Dioxolane Dipentaerythritol	(HOCH ₂) ₃ CCH ₂ OCH ₂ - C(CH ₂ OH) ₃	74.08 254.28	19 ² , 3	1.060 ²⁰	1.4000 ²⁰	-95 215-218	74–75	<1	misc aq; s alc, eth
d649	Dipentene	(6112611)3	136.24	5, 137	0.8402_4^{21}	1.4739^{20}		176	42	i ag; misc alc
d650	Dipentylamine	(C ₅ H ₁₁) ₂ NH	157.29	4 ¹ , 378	0.777	1.4272		195-202	39	v s alc, eth
d651	Dipentyl ether	$(C_5H_{11})_2O$	158.29	1 ¹ , 193	0.7833_4^{20}	1.4120^{20}	-69.4	186.8	63	misc alc, eth; s
										acet
d652	Diphenylacetic acid	(C ₆ H ₅) ₂ CHCOOH	212.25	9, 673	1.25815		148	195 ^{5mm}		s hot aq, alc, chl,
d653	Diphenylacetonitrile	(C ₆ H ₅) ₂ CHCN	193.25	9, 674			76	181 ^{12mm}		s alc, eth
d654	Diphenylacetylene	$C_6H_5C\equiv CC_6H_5$	178.23	5,656	0.990		60–61	300		v s hot alc, eth
d655	Diphenylamine	$(C_6H_5)_2NH$	169.23	12, 174	1.160		53–54	302	152	45 alc; v s bz, eth
d656	cis,cis-1,4-	C ₆ H ₅ CH=CH-	206.29	5, 676	0.9697_4^{101}	1.6347101	70.5	502	102	s bz, chl, eth, PE
	Diphenyl-1,3-buta- diene	CH=CHC ₆ H ₅		-, -, -	4	(He line)	,			2 2 -, 2 2 2 , 2 2 2 , 2 2 2
d657	cis,trans-1,4- Diphenyl-1,3- diene	C ₆ H ₅ CH=CH- CH=CHC ₆ H ₅	206.29	5, 676	0.9974422	1.6053 ²²	88	133 ^{0.1mm}		s alc, bz, eth, chl
d658	1,3-Diphenyl-2-	$C_{\epsilon}H_{\epsilon}C(O)CH=$	222.27	$7^2,433$	1.108045	1.634320	-30	246 ^{50mm}		i ag; s alc, eth
4050	buten-1-one	$C(C_6H_5)CH_3$, , 133	1.10004	1.03 13	glass	210		ruq, sure, em
d659	Diphenylcarbamoyl chloride	$(C_6H_5)_2NCOC1$	231.68				82–84			
d660	1,5-Diphenylcarbo- hydrazide	$(C_6H_5NHNH)_2C=O$	242.28	15, 292			168–171			s hot alc, acet, HOAc
d661	Diphenyl carbonate	$(C_6H_5O)_2C=O$	214.22	6, 158			80-81	302-306		s hot alc, bz, eth
d662	Diphenyl chloro- phosphate	$(C_6H_5O)_2P(O)Cl$	268.64	6, 179	1.296	1.5500 ²⁰		314 ^{272mm}	>112	

d663	Diphenyl diselenide	C ₆ H ₅ SeSeC ₆ H ₅	312.13	6,346	1.557_4^{80}		61–64	210		s hot alc
d664	Diphenyl disulfide	$C_6H_5SSC_6H_5$	218.34	6, 323	1.353_4^{20}		58–60	310		s alc, bz, eth; i aq
d665	Diphenylenimine		167.21	20, 433	1.10^{18}_{4}		246	355		0.8 bz; 3 eth; 16
										pyr; 11 acet; i
										aq
d666	1,2-Diphenylethane	C ₆ H ₅ CH ₂ CH ₂ C ₆ H ₅	182.27	5, 598	0.995_4^{20}	1.5338	52.5	284		s alc; v s chl, eth
d667	Diphenyl ether	C ₆ H ₅ OC ₆ H ₅	170.21	6, 146	1.0661_4^{20}	1.5763^{30}	26.9	258.3	115	s alc, bz, eth,
		-03 - 03		,,,,,,,						HOAc
d668	1,2-Diphenylethyl-	$C_6H_5CH_2CH(C_6H_5)NH_2$	197.28	12, 1326	1.020	1.5802^{20}		311	>112	
	amine	-6 3 - 2 - (-6 3) - 2		,						
d669	<i>N</i> , <i>N</i> ′-Diphenylethyl-	C ₆ H ₅ NHCH ₂ CH ₂ NHC ₆ H ₅	212.30	12, 543			67.5	228-330		v s alc, eth
	enediamine									
d670	N,N'-Diphenyl-	C ₆ H ₅ N=CHNHC ₆ H ₅	196.25	12, 236			138-141			s eth; v s chl
	formamidine			,						,
d671	1,3-Diphenyl-	$C_6H_5NHC(=NH)NHC_6H_5$	211.27	12, 369	1.13		150	d 170		s alc, hot bz, chl
	guanidine									

3,6-Dioxa-1,8-octanediol, t270

4,8-Dioxa-1,11-undecanediol, t408

(2,5-Dioxo-4-imidazolidinyl)urea, a77

1,3-Dioxolane-2-one, e124

3,4-Dioxypentane, d439

Dipentyl ketone, u6

Diphenic acid, b137 Diphenylacetone, d684 Diphenylcarbamyl chloride, d659 sym-Diphenylcarbazide, d660 Diphenyldiazone, a322 Diphenylethanedione, b34 Diphenylethanedione dioxime, b35 1,2-Diphenylethene, s9 Diphenylethyne, d654 Diphenylglycolic acid, b36 Diphenylglyoxime, b35

 CH_3

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d672	5,5-Diphenyl- hydantoin		252.27	24, 410			295–298			i aq; 1.7 alc; 3.3 acet
d673	1,2-Diphenyl- hydrazine	C ₆ H ₅ NHNHC ₆ H ₅	184.24	15, 123	1.15846		123–126			v s alc; sl s bz
d674	Diphenyl isooctyl- phosphite	$(CH_3)_2CH(CH_2)_5PH-$ $(OC_6H_5)_2$	346.40		1.044	1.522				
d675	Diphenylmercury	$(C_6H_5)_2Hg$	354.81	16, 946	2.318^{4}		124-125	d > 306		s chl; sl s hot alc
d676	Diphenylmethane	$C_6H_5CH_2C_6H_5$	168.24	$5^2,498$	1.3421_4^{10}	1.5768	25.9	264.5	>112	v s alc, bz, chl, eth
d677	Diphenylmethanol	$(C_6H_5)_2$ CHOH	184.24	6, 678			66.7	298		0.05 aq; v s alc, chl, eth
d678	1,1-Diphenylmethyl- amine	$C_6H_5CH(NH_2)C_6H_5$	183.25	12, 1323	1.0635 ₄ ²² super-cooled	1.595699	34	295	>112	sl s aq
d679	2,5-Diphenyloxazole		221.26	27, 78			72–73	360		
d680	2,6-Diphenylphenol	$(C_6H_5)_2C_6H_3OH$	246.31	6 ³ , 3631			100-102			
d681	Diphenyl phosphite	$(C_6H_5O)_2P(=O)H$	234.19	6 ¹ , 94	1.223	1.5575^{20}	12	219 ^{26mm}	176	
d682	Diphenylphosphoryl azide	$(C_6H_5O)_2P(=O)N_3$	275.20		1.277	1.5518 ²⁰		157 ^{0.17mm}	>112	
d683	2,2-Diphenyl-1- picrylhydrazyl		394.32	$16^2, 363$			127 d			
d684	1,3-Diphenyl-2- propanone	$C_6H_5CH_2C(=O)$ - $CH_2C_6H_5$	210.28	7, 445	1.2		32–34	330		i aq; v s alc, eth
d685	1,3-Diphenyl-2- propen-1-one	$C_6H_5CH=CHC(=0)$ - C_6H_5	208.26	7, 478	1.0712_4^{62}	1.6458 ⁶²	57–58	208 ^{25mm}		v s bz, chl, eth
d686	2,2-Diphenyl- propionic acid	$CH_3C(C_6H_5)_2COOH$	226.28	9 ² , 474			175–177	300		s alc; v s bz, eth
d687	Diphenylsilanediol	$(C_6H_5)_2Si(OH)_2$	216.31	16, 909			140 d		53	
d688	Diphenyl sulfide	$(C_6H_5)_2S$	186.28	6, 299	1.11815	1.632720	-40	296	>112	misc bz, eth, CS ₂
d689	Diphenyl sulfone	$(C_6H_5)_2SO_2$	218.27	6, 300	-15		128–129	379		i aq; s hot alc, bz

d690	Diphenyl sulfoxide	$(C_6H_5)_2S=0$	202.28 256.33	6,300			69–71 168 d	207 ^{13mm}		i agaya ahl CCl
d691	Diphenylthio- carbazone	$C_6H_5N=NC(S)NH-NHC_6H_5$	230.33	16, 26			108 0			i aq; v s chl, CCl ₄
d692	1,3-Diphenylthio- urea	C ₆ H ₅ NHC(S)NHC ₆ H ₅	228.32	12, 394	1.32		154			i aq; v s alc, eth
d693	1,3-Diphenylurea	C ₆ H ₅ NHC(O)NHC ₆ H ₅	212.25	12, 352	1.239		238	260 d		0.015 aq; s eth, HOAc
d694	1,2-Dipiperidino- ethane		196.34	20 ¹ , 19	0.916	1.4876 ²⁰	-0.5	265	110	поас
d695	Dipiperidinomethane		182.31		0.915	1.4820^{20}		123 ^{15mm}		
d696	Dipropylamine	$(C_3H_7)_2NH$	101.19	4, 138	0.7375_4^{20}	1.4043 ²⁰	-39.6	109.2	17	4 aq; v s alc, eth, PE
d697	Dipropylene glycol butyl ether	CH ₃ CH(OH)CH ₂ OCH ₂ - CH(OC ₄ H ₉)CH ₃	190.3		0.917_{25}^{25}	1.425 ²⁵		229	113	

5,5-Diphenyl-2,4-imidazolidinedione, d672 Diphenyl ketone, b53 Diphenyl oxide, d667 Diphenylphosphorochloridate, d662 1,3-Diphenyl-1,3-propanedione, d53 sym-Diphenylthiourea, t146 Dipicolinic acid, p261 Di-2-propenylamine, d25

d683

Dipropyl adipate, d702 Dipropylene glycol, h172

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d698	Dipropylene glycol	CH ₃ CH(OH)CH ₂ OCH ₂ -	162.2		0.930_{25}^{25}	1.419 ²⁵		388	90	
d699	ethyl ether Dipropylene glycol isopropyl ether	CH(OC ₂ H ₅)CH ₃ CH ₃ CH(OH)CH ₂ OCH ₂ - CH[OCH(CH ₃) ₃]CH ₃	176.2		0.878_{25}^{25}	1.421 ²⁵		80.1	90	
d700	Dipropylene glycol methyl ether	CH ₃ CH(OH)CH ₂ OCH ₂ - CH(OCH ₃)CH ₃	148.2		0.95120	1.419 ²⁰	-117	188.3	85	
d701	Dipropyl ether	$(C_3H_7)_2O$	102.18	1,354	0.7466^{20}	1.3803 ²⁰	-123.2	89.6	4	0.4 aq
d702	Dipropyl hexane- dioate	C ₃ H ₇ OOC(CH ₂) ₄ - COOC ₃ H ₇	230.30	$2^2,574$	0.9790_4^{20}	1.4314 ²⁰	-20	144 ^{10mm}		i aq; s alc, eth
d703	Dipropyl sulfate	$(C_3H_7O)_2SO_2$	182.24	1,354	1.106_4^{20}		d 140	120 ^{20mm}		v s PE
d704	Dipropyl sulfone	$(C_3H_7)_2SO_2$	150.24	1,359	1.028_4^{50}		28-30	270	126	
d705	2,2'-Dipyridyl		156.19	23, 199			69.7	273		0.5 aq; v s alc, bz, chl, eth, PE
d706	2,2'-Dipyridylamine		171.20	221,630			89–90	222 ^{50mm}		, , , ,
d707	1,3-Dithiane		120.24	-			53-55		90	
d708	4,4'-Dithiobutyric acid	HOOC(CH ₂) ₃ SS(CH ₂) ₃ - COOH	238.32	3, 312			110			
d709	3,3'-Dithiopropionic acid	HOOCCH ₂ CH ₂ SSCH ₂ - CH ₂ COOH	210.27				157–159			
d710	Dithiooxamide	$H_2NC(=S)C(=S)NH_2$	120.20	2, 565			170 d	subl		sl s aq; s alc; i eth
d711	1,3-Di- <i>o</i> -tolyl- guanidine	$(CH_3C_6H_4NH)_2C=NH$	239.32	12, 803	1.10_4^{20}		176–178			s hot alc, eth
d712	1,5-Di(vinyloxy)-3- oxapentane	(CH ₂ =CHOCH ₂ CH ₂) ₂ O	158.20		0.975^{29}	1.445		81 ^{10mm}		
d713	1,3-Divinyltetra- methyldisiloxane	[CH ₂ =CHSi(CH ₃) ₂] ₂ O	186.39		0.811_4^{20}	1.41220	-99.7	139		
d714	3,9-Divinyl-2,4,8,10- tetraoxaspiro[5.5]-		212.25		1.251		40–54	120 ^{2mm}	110	
	undecane									

d715 d716 d717	Docosane Docosanoic acid 1-Docosanol	CH ₃ (CH ₂) ₂₀ CH ₃ CH ₃ (CH ₂) ₂₀ COOH CH ₃ (CH ₂) ₂₁ OH	310.61 340.60 326.61	1, 174 2, 391 1, 431	$\begin{vmatrix} 0.7782^{45} \\ 0.8221_4^{100} \end{vmatrix}$	1.4358 ⁴⁵ 1.4270 ¹⁰⁰	44.4 80–82 65–72	369 206 ^{60mm} 180 ^{0.22mm}		i aq; sl s alc; v s eth 0.2 alc; 0.19 eth sl s eth; s alc, chl
d718	1H, <i>H</i> , 7 <i>H</i> - Dodeca-fluoro-1-heptanol	HCF ₂ (CF ₂) ₅ CH ₂ OH	332.0		1.7616^{20}	1.3180^{20}		169–170		
d719 d720	Dodecane 1,12-Dodecanediamine	CH ₃ (CH ₂) ₁₀ CH ₃ H ₂ N(CH ₂) ₁₂ NH ₂	170.41 200.37	1, 171 4, 273	0.7490_4^{20}	1.4216^{20}	-9.6 62-65	216.28	71 155	
d721	Dodecanedioic acid	$HOOC(CH_2)_{10}COOH$	230.30	2,729			128–130	245 ^{10mm}	133	
d722	1,2-Dodecanediol	CH ₃ (CH ₂) ₉ CH(OH)- CH ₃ OH	202.34	$1^3, 2237$			58–60			
d723	1,12-Dodecanediol	HOCH ₂ (CH ₂) ₁₀ CH ₂ OH	202.34	1 ² , 562			81-84	189 ^{12mm}		
d724	Dodecanenitrile	CH ₃ (CH ₂) ₁₀ CN	181.32	2, 363	0.827	1.4360^{20}		198 ^{100mm}	>112	misc alc, bz, chl, eth
d725	1-Dodecanethiol	CH ₃ (CH ₂) ₁₁ SH	202.40		0.845_{20}^{20}	1.4587^{20}		266–283	87	i aq; s alc, eth
d726	Dodecanoic acid	CH ₃ (CH ₂) ₁₀ COOH	200.32	2, 359	0.8694	1.418382	44	225 ^{100mm}		i aq; 100 alc; v s bz, eth
d727 d728	1-Dodecanol Dodecanoyl chloride	CH ₃ (CH ₂) ₁₁ OH CH ₃ (CH ₂) ₁₀ COCl	186.34 218.77	1, 428 2, 363	0.8308_4^{25} 0.946	$1.4413^{25} 1.4459^{20}$	23.8	259 134 ^{11mm}	>112 >112	i aq; s alc, eth
d729	1-Dodecene	$CH_3(CH_2)_9CH=CH_2$	168.32	1, 225	0.7584_4^{20}	1.4294^{20}	-35.2	213.4	77	s alc, eth, PE

Dipropyl ketone, h17 Distearylpentaerythritoldiphosphite, b196 Disulfiram, t61 2,3-Dithiabutane, d516 5,6-Dithiadecane, d113 3,4-Dithiahexane, d294 2,2'-Dithiodiethanol, h118 1,4-Dithiothreitol, d424 Dithizone, d691 Divinylene oxide, f40 DMSO, d614 Dodecyl alcohol, d727

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d730	2-Dodecen-1-yl- succinic anhydride		266.38					180 ^{5mm}	177	
d731 d732	Dodecanal Dodecylamine	CH ₃ (CH ₂) ₁₀ CHO CH ₃ (CH ₂) ₁₁ NH ₂	184.32 185.36	1,714 4,200	0.835	1.4344 ²⁰	28–30	185 ^{100mm} 247–249	101 >112	misc alc, bz, chl,
d733	4-Dodecylaniline	CH ₃ (CH ₂) ₁₁ C ₆ H ₄ NH ₂	261.46	12 ³ , 2776			40–41	220– 221 ^{15mm}		
d734 d735	Dodecylcyclohexane Dodecyl sulfate, Na salt	CH ₃ (CH ₂) ₁₁ C ₆ H ₁₁ CH ₃ (CH ₂) ₁₁ OSO ₃ ⁻ Na ⁺	252.50 288.38		0.8250	1.4580 ²⁰	12 204–207	131 ^{0.8mm}		10 aq
d736	Dodecyltrichloro- silane	CH ₃ (CH ₂) ₁₁ SiCl ₃	303.8			1.458 ²⁰		155 ^{10mm}		
d737 d738	Dotriacontane Dulcitol	CH ₃ (CH ₂) ₃₀ CH ₃	450.88 182.17	1, 177 1, 544	$0.8124_4^{20} \\ 1.47^{20}$	1.4364 ⁷⁰	68–70 188–189	467 275 ^{1mm}		sl s alc, bz, eth 3.3 aq; sl s alc
e1	D-Ephedrine	CH ₃ NHCH(CH ₃)CH(OH)- C ₆ H ₅	165.24	13, 637			119	225		v s alc, eth
e2	L-Ephedrine	CH ₃ NHCH(CH ₃)CH(OH)- C ₆ H ₅	165.24	13, 636			34	255		5 aq; v s alc; s chl
e3	1,2-Epoxybutane	CH ₃ CH ₂ CH—CH ₂	72.11	17 ² , 17	0.829720	1.3840 ²⁰	-150	63.2	-17	6 aq; misc alc, bz, chl, eth
e4	1,2-Epoxycyclo- dodecane	0	182.31		0.939	1.4773 ²⁰				
e5	1,2-Epoxycyclo- hexane		98.15	17, 21	0.970	1.4520 ²		129–130	27	v s alc, bz, eth
e6 e7	1,4-Epoxycyclohexane 2-(3,4-Epoxycyclohexyl)ethyltrimethoxysilane		98.15 246.37		0.969 1.070 ₄ ²⁵	1.4480 ²⁰ 1.449 ²⁵		119 ^{713mm} 310	12 146	

e7a 1,2-Epoxyc	yclooctane	126.20				53-56	55 ^{5mm}	56	
e8 1,2-Epoxyc	yclo-	84.12	17, 21	0.964	1.4336^{20}		102	10	
pentane									
e9 1,2-Epoxye	thyl- C ₆ H ₅ CH—CH ₂	120.15	17, 49	1.0523_4^{16}	1.5338^{20}	-37	194	79	i aq; s alc, eth
benzene									
e9a 1,2-Epoxy-	$G_{\circ}^{\text{phenoxy}} \mid C_{\circ}^{\text{H}} \cap C_{\circ}^{\text{H}} \cap C_{\circ}^{\text{H}}$	CH ₂ 150.18				2			
propane		· •							
e10 1,2-Epoxyp	ropane CH ₃ CH-CH ₂	58.08	17, 6	0.859_4^0	1.3660^{20}	-112.1	34.2	-37	41 aq; misc alc,
									eth
e11 2,3-Epoxy-	1-propanol O H ₂ C—CHCH ₂ OH	74.08	17, 104	1.1143_4^{25}	1.4315^{20}		66 ^{2.5mm}	81	misc aq

Dodecyl aldehyde DPPH, d683 Durene, t99 Durenol, t116 EDTA, e125 Eicosane, i2 1-Eicosene, i3 Elaidic acid, o11 Embonic acid, m235 Enanthic acid, h10 Epibromohydrin, b276 Epichlorohydrin, c101 1,4-Epoxybutane, t66 Epoxyethane, e129 1,3-Epoxypropane, t345

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e12	2,3-Epoxypropyl methacrylate	H ₂ C=C(CH ₃)COO- CH ₂ CH-CH ₂	142.15		1.042	1.449420		189	83	
e13	1,2-Epoxy-3,3,3-tri- chloropropane	CH ₂ CH—CH ₂	161.42	17 ² , 14	1.495	1.477820		151 ^{745mm}	66	
e14	Ethane	CH ₃ CH ₃	30.07	1,80	0.5462, ⁻⁸⁸ 1.0493 ₄ ⁰ , g·L		-183.3	-88.6		4.7 mL aq; 46 mL alc ⁴
e15	1,2-Ethanediamine	H,NCH,CH,NH,	60.10	4, 230	0.8977_4^{20}	1.4568 ²⁰	8.5	117.3	33	misc aq, alc; i bz
e16	1,2-Ethanediol	HOCH ₂ CH ₂ OH	62.07	1, 465	1.1135_4^{20}	1.4318 ²⁰	-12.6	197.3	110	misc aq, alc, glyc,
e17	1,2-Ethanediol diacetate	CH ₃ COOCH ₂ CH ₂ OOCCH ₃	146.14	2, 142	1.1043 ²⁰	1.4150 ²⁰	-31	190.2	82	misc alc, eth
e18	1,2-Ethanedithiol	HSCH ₂ CH ₂ SH	94.20	1,471	1.123^{24}	1.5580^{20}		146	50	v s alc, alk
e19	Ethanesulfonyl chloride	CH ₃ CH ₂ SO ₂ Cl	128.57	$4^2,526$	1.357 ²²	1.433920		171		d aq, alc; v s eth
e20	Ethanethiol	CH ₃ CH ₂ SH	62.13	1,340	0.8315^{25}	1.420^{25}	-147.9	35.0	-17	0.7 aq; s alc, eth
e21	Ethanol	CH ₃ CH ₂ OH	46.07	1, 292	0.7894_4^{20}	1.3614 ²⁰	-114.5	78.3	8	misc aq, alc, eth,
e22	Ethanol-d	CH ₃ CH ₂ OD	47.08	1 ³ , 1287	0.801	1.3595^{20}		78.8	12	misc aq, alc, eth
e23	Ethoxyacetic acid	CH ₃ CH ₂ OCH ₂ COOH	104.11	3, 233	1.1021_4^{20}	1.4190^{20}		97 ^{11mm}	97	s aq, alc, eth
e24	4-Ethoxyaniline	CH ₃ CH ₂ OC ₆ H ₄ NH ₂	137.18	13, 436	1.0652_4^{16}	1.5609^{20}	4	250	115	i aq; s alc
e25	2-Ethoxybenzaldehyde	CH ₃ CH ₂ OC ₆ H ₄ CHO	150.18	8, 43	1.074	1.5422^{20}	20	136 ^{24mm}	107	misc alc, eth
e26	4-Ethoxybenzaldehyde	CH ₃ CH ₂ OC ₆ H ₄ CHO	150.18	8, 73	1.080_{25}^{25}	1.5584^{20}	13–14	255	>112	v s alc, bz, eth
e27	2-Ethoxybenzamide	CH ₃ CH ₂ OC ₆ H ₄ CONH ₂	165.19	10, 93			132–133			sl s aq; s alc, eth
e28	Ethoxybenzene	CH ₃ CH ₂ OC ₆ H ₅	122.17	6, 140	0.967 ₄ ²⁰	1.5074 ²⁰	-29.5	170.0		0.12 aq; misc alc, eth
e29	2-Ethoxybenzoic acid	CH ₃ CH ₂ OC ₆ H ₄ COOH	166.18	10, 64	1.105	1.5400 ²⁰	19.4	174 ^{15mm}	>112	sl s aq

20	14 54 1 1 11		166.10	10 156	ı	ı	107 100	ı		. 1 1 .
e30	4-Ethoxybenzoic acid	CH ₃ CH ₂ OC ₆ H ₄ COOH	166.18	10, 156		1 522120	197–199	265		sl s hot aq
e31	2-Ethoxybenzyl alcohol	CH ₃ CH ₂ OC ₆ H ₄ CH ₂ OH	152.19	6, 893		1.5321 ²⁰		265		
e32	Ethoxycarbonyl isothiocyanate	CH ₃ CH ₂ OC(=O)NCS	131.15	3 ³ , 279	1.112	1.5000^{20}		56 ^{18mm}	50	
e33	Ethoxydimethylvinyl-silane	$(CH_3)_2Si(OC_2H_5)-$ $CH=CH_2$	130.3		0.790_4^{20}	1.39820		99 ^{710mm}		
e34	2-Ethoxyethanol	CH ₃ CH ₂ OCH ₂ CH ₂ OH	90.12	1,467	0.929520	1.4075^{20}	-59	134.8	48	misc aq, alc, eth, acet
e35	2-(2-Ethoxyethoxy)- ethanol	C ₂ H ₅ OCH ₂ CH ₂ OCH ₂ - CH ₂ OH	134.18	1 ² , 520	0.9841425	1.4254 ²⁵	-55	201.9	96	misc aq, alc, bz, chl, acet, pyr
e36	2-(2-Ethoxyethoxy)- ethyl acetate	C ₂ H ₅ OCH ₂ CH ₂ OCH ₂ - CH ₂ OOCCH ₃	176.21		1.0096 ²⁰	1.4213 ²⁰	-25	218.5	110	misc aq, alc, eth, oils
e37	2-Ethoxyethyl acetate	CH ₃ COOCH ₂ CH ₂ - OCH ₂ CH ₃	132.16	2 ² , 155	0.9749_4^{20}	1.4023 ²⁰	-61.7	156.3	57	29 aq; misc alc, eth
e38	2-Ethoxyethylamine	CH ₃ CH ₂ OCH ₂ CH ₂ NH ₂	89.14	$4^2,718$	0.8512_4^{20}	1.4101^{20}		107	21	misc aq, alc, eth
e39	3-Ethoxy-4-hydroxy- benzaldehyde	C ₂ H ₅ OC ₆ H ₃ (OH)CHO	166.18	8, 256			76–78			s eth, glycols; 50 alc
e40	3-Ethoxymethacrolein	C ₂ H ₅ OCH=C(CH ₃)CHO	114.15	14, 4082	0.960	1.479220		78- 81 ^{14mm}	35	
e41	4-Ethoxy-3-methoxy- benzaldehyde	C ₂ H ₅ OC ₆ H ₃ (OCH ₃)CHO	180.20	8, 256			59–60			s alc, bz, chl, eth
e42	Ethoxymethyldi- phenylsilane	$(C_6H_5)_2Si(CH_3)OC_2H_5$	242.4		1.018_4^{20}	1.544 ²⁰		122 ^{0.3mm}		
e43	Ethoxymethylene- malononitrile	CH ₃ CH ₂ OCH=C(CN) ₂	122.13	3 ¹ , 162			64–66	160 ^{12mm}		

Eschenmoser's salt, d549 Estragole, a94 Ethanal, a4 Ethanediamide, o54 Ethanenitrile, a29 Ethanoic acid, a19 Ethanolamine, a164 Ethenyl acetate, v2 Ethenylbenzene, s19 4-Ethoxy-*m*-anisaldehyde, e41 1-Ethoxybutane, b449 Ethoxyethane, d300 2-Ethoxyethyl ether, b176 Ethoxyformic anhydride, d326

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e44 e45	1-Ethoxynaphthalene N-(4-Ethoxyphenyl)- acetamide	C ₁₀ H ₇ OCH ₂ CH ₃ CH ₃ CH ₂ OC ₆ H ₄ NHCOCH ₃	172.23 179.21	6, 606 13 ² , 244	1.060420	1.6040 ²⁰	5.5 134–135	280	>112	i aq; v s alc, eth 0.076 aq; 6.7 alc; 7.1 chl; 1.1 eth; s glyc
e46	trans-2-Ethoxy-5- (1-propenyl)phenol	C ₂ H ₅ OC ₆ H ₃ (CH=CH- CH ₃)OH	178.23	6 ² , 918						
e47	3-Ethoxypropylamine	C,H,OCH,CH,CH,NH,	103.17	$4^3,739$	0.861	1.4178^{20}		136-138	32	
e48	3-Ethoxysalicyl- aldehyde	C ₂ H ₅ OC ₆ H ₃ (OH)CHO	166.18	$8^2, 267$			86–88	263–264		
e49	2-Ethoxytetrahydro- furan	$C_2H_5O(C_4H_7O)$	116.16	174, 1020	0.908	1.4140 ²⁰		170–172	16	
e50	Ethoxytrimethyl- silane	(CH ₃) ₃ SiOC ₂ H ₅	118.3		0.7573_4^{20}	1.374220				
e51	Ethyl acetate	CH ₃ COOC ₂ H ₅	88.11	2, 125	0.9006_4^{20}	1.3724 ²⁰	-84	77.1	-3	9.7 aq; misc alc, acet, chl, eth
e52	Ethyl acetimidate HCl	$CH_3C(=NH)OC_2H_5 \cdot HCl$	123.58	2, 182			112–114			
e53	Ethyl acetoacetate (enol)	CH ₃ COCH=C(OH)OC ₂ H ₅	130.15	3, 632	1.011910	1.448010	-44	180.8	84	1.9 aq; misc alc, chl
e54	Ethyl acetoacetate (keto)	CH ₃ COCH ₂ COOC ₂ H ₅	130.15	3, 632	1.036810	1.422410	-39	180.8	84	12 aq; misc alc, chl
e55	p-Ethylacetophenone	C ₂ H ₅ C ₆ H ₄ COCH ₃	148.21	7 ⁴ , 1101	0.993	1.5293^{20}	-20.6	114 ^{11mm}	90	
e56	Ethyl acrylate	CH ₂ =CHCOOCH ₂ CH ₃	100.12	2, 399	0.9405_4^{20}	1.4068^{20}	-71.2	99.5	15	1.5 aq; s alc, eth
e57	Ethylaluminum dichloride	CH ₃ CH ₂ AlCl ₂	126.95		1.207 ⁵⁰		32	113 ^{50mm}		_
e58	Ethylamine	CH ₃ CH ₂ NH ₂	45.09	4, 87	0.689_{15}^{15}		-81.0	16.6	-17	misc aq, alc, eth
e59	Ethyl 2-amino- benzoate	H ₂ NC ₆ H ₄ COOCH ₂ CH ₃	165.19	14, 319	1.08815		14	266–268		i aq; s alc, eth

e60	Ethyl 4-amino- benzoate	H ₂ NC ₆ H ₄ COOCH ₂ CH ₃	165.19	14, 422			88–90	310		0.04 aq; 20 alc; 50 chl; 25 eth; s dil acid
e61	Ethyl 3-amino- crotonate	CH ₃ C(NH ₂)=CH- COOCH ₂ CH ₃	129.16	3, 654	1.021_4^{20}		33–35	210–215		i aq; s alc, bz, eth
e62	2-(Ethylamino)- ethanol	CH ₃ CH ₂ NHCH ₂ CH ₂ OH	89.14	4, 282	0.914_4^{20}	1.4402^{20}	-90	170	71	v s aq, alc, eth
e63	N-Ethylaniline	C ₆ H ₅ NHCH ₂ CH ₃	121.18	12, 159	0.958^{25}_{25}	1.5559^{20}	-63	204.5	85	i ag; misc alc, eth
e64	2-Ethylaniline	CH ₃ CH ₂ C ₆ H ₄ NH ₂	121.18	12 ² , 584	0.983_4^{22}	1.5590^{20}	-44	210	97	sl s ag; v s alc, eth
e65	4-Ethylaniline	CH ₃ CH ₂ C ₆ H ₄ NH ₂	121.18	12, 1090	0.975_4^{22}	1.5542^{20}	-5	216	85	sl s aq; v s alc, eth
e66	2-Ethylanthraquinone	32-64- :2	236.27	7 ¹ , 425			108–111			
e67	Ethylbenzene- d_{10}	C ₆ D ₅ CD ₂ CD ₃	116.25	' ', '		1.4920^{20}		134.6	31	
e68	Ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	106.17	5 ² , 274	0.8670_4^{20}	1.4959^{20}	-95.0	136.2	20	0.01 aq; misc alc, bz, chl, eth
e69	Ethyl benzoate	C ₆ H ₅ COOCH ₂ CH ₃	150.18	9, 110	1.050_4^{25}	1.5052^{20}	-34.7	212.4	84	0.05 aq; misc alc, chl, bz, eth, PE
e70	Ethyl benzoylacetate	C ₆ H ₅ C(=O)CH ₂ - COOCH ₂ CH ₃	192.21	10, 674	1.110	1.5338 ²⁰		265 d	140	i aq; misc alc, eth
e71	Ethyl 2-benzylaceto- acetate	CH ₃ COCH(CH ₂ C ₆ H ₅)- COOC ₂ H ₅	220.27	10, 674	1.036	1.4996 ²⁰		276	>112	
e72	N-Ethylbenzylamine	C ₆ H ₅ CH ₂ NHC ₂ H ₅	135.21	12, 1020	0.909	1.5117^{20}		194	66	
e73	Ethyl (2-benzyl)- benzoylacetate	C ₆ H ₅ COCH(CH ₂ C ₆ H ₅)- COOC ₂ H ₅	282.34	10, 764	1.110	1.5567 ²⁰		270 ^{80mm}	>112	

 α -Ethoxy- α -phenylacetophenone, b47

3-Ethoxy-1-propene, a90

Ethyl alcohols, e21, e22

Ethylaldehyde, a4 Ethyl anthranilate, e59 Ethyl benzenecarboxylate, e69 Ethyl 3-benzenepropenoate, e103 α -Ethylbenzyl alcohol, p142

$$C_2H_5$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e74	Ethyl N-benzyl-N- cyclopropyl- carbamate	C ₆ H ₅ CH ₂ N(C ₃ H ₅)- COOCH ₂ CH ₃	219.28		0.997	1.5104 ²⁰			>112	
e75	Ethyl bromoacetate	BrCH ₂ COOCH ₂ CH ₃	167.01	2, 214	1.506_{20}^{20}	1.4510^{20}		159	47	i aq; misc alc, eth
e76	Ethyl 2-bromo-	CH ₃ CH ₂ CH(Br)-	195.06	$2^2, 255$	1.329_{20}^{20}	1.4470^{20}		177 d	58	i aq; misc alc, eth
	butyrate	COOCH ₂ CH ₃								-
e77	Ethyl 4-bromo-	BrCH ₂ CH ₂ CH ₂ -	195.06	2, 283	1.363	1.4559^{20}		82 ^{10mm}	90	
	butyrate	COOCH ₂ CH ₃								
e78	Ethyl 2-bromoiso-	(CH ₃) ₂ C(Br)-	195.06	2, 296	1.329_4^{20}	1.4446^{20}		67 ^{11mm}	60	i aq; misc alc, eth
	butyrate	COOCH ₂ CH ₃								
e79	Ethyl 3-bromo-2-oxo-	$BrCH_2C(=O)$ -	195.02	$3^2,409$	1.554	1.4695^{20}		100 ^{10mm}	98	
	propionate	COOCH ₂ CH ₃								
e80	Ethyl 2-bromo-	CH ₃ (CH ₂) ₂ CH(Br)-	209.09	2,302	1.226	1.4486^{20}		190–192	77	i aq; misc alc, eth
	pentanoate	COOCH ₂ CH ₃								
e81	Ethyl 2-bromopro-	CH ₃ CH(Br)COOCH ₂ CH ₃	181.03	2, 255	1.447_{20}^{20}	1.4470^{20}	159–160	51		i aq; misc alc, eth
	pionate				10					
e82	Ethyl 3-bromopro-	BrCH ₂ CH ₂ COOCH ₂ CH ₃	181.03	2, 256	1.4123_4^{18}	1.4569^{18}		136 ^{50mm}	79	i aq; misc alc, eth
	pionate									
e83	2-Ethyl-1-butanol	(C ₂ H ₅) ₂ CHCH ₂ OH	102.18	1,412	0.8330^{20}	1.4224^{20}	-114.4	146.5	58	0.63 aq
e84	2-Ethyl-1-butene	$(C_2H_5)_2C=CH_2$	84.16	$1^3,814$	0.6696_4^{20}	1.3967^{20}	-131.5	64.7		
e85	<i>N</i> -Ethylbutylamine	CH ₃ (CH ₂) ₃ NHCH ₂ CH ₃	101.19	4, 157	0.740_4^{20}	1.4050^{20}		108	18	
e86	2-Ethylbutylamine	$(C_2H_5)_2CHCH_2NH_2$	101.19	4, 192	0.776_{20}^{20}			121–125	21	s aq, alc, acet, eth
e87	2-Ethylbutyraldehyde	(C ₂ H ₅) ₂ CHCHO	100.16	1, 693	0.8162_{20}^{20}	1.4018^{20}	-89	116.7	21	0.31 aq
e88	Ethyl butyrate	CH ₃ CH ₂ CH ₂ COOCH ₂ CH ₃	116.16	2, 270	0.879_4^{20}	1.3928^{20}	-98.0	121.6	29	0.49 aq; misc alc,
					20					eth
e89	2-Ethylbutyric acid	(C ₂ H ₅) ₂ CHCOOH	116.16	2, 333	0.9225_{20}^{20}	1.4133^{20}	-15	194.2	99	0.22 aq
e90	Ethyl butyrylacetate	CH ₃ (CH ₂) ₂ C(O)CH ₂ -	158.20	3, 684	1.001	1.4295^{20}		104 ^{22mm}	78	
		COOC ₂ H ₅								

e91	Ethyl carbamate	H ₂ NCOOCH ₂ CH ₃	89.09	3,22	1.056		49–50	182-184		200 aq; 125 alc;
										111 chl; 67 eth
e92	Ethyl carbazate	H ₂ NNHCOOCH ₂ CH ₃	104.11	3,98			44-47	110 ^{22mm}		
e93	N-Ethylcarbazole		195.27	20, 436			66–68			
e94	Ethyl chloroacetate	ClCH ₂ COOCH ₂ CH ₃	122.55	2, 197	1.1498_4^{20}	1.4227^{20}	-26	144-146	65	i aq; misc alc, eth
e95	Ethyl 2-chloroaceto-	CH ₃ C(=O)CH(Cl)-	164.59	3,662	1.190	1.4430^{20}		107 ^{14mm}	50	i aq; s alc, eth
	acetate	COOC ₂ H ₅								_
e96	Ethyl 4-chloroaceto-	$ClCH_2C(=O)CH_2$	164.59	3,663	1.218_4^{17}	1.4520^{20}		115 ^{14mm}	96	i aq; misc alc, eth
	acetate	COOC ₂ H ₅								_
e97	Ethyl 4-chloro-	CICH ₂ CH ₂ CH ₂ COOC ₂ H ₅	150.61	2, 278	1.0754_4^{20}	1.4306^{20}		186	51	s alc, acet, eth
	butyrate									
e98	Ethyl chloroformate	ClCOOC ₂ H ₅	108.52	3, 10	1.1403_4^{20}	1.3941^{20}	-81	95	2	misc alc, bz, chl,
										eth
e99	Ethyl 2-chloropro-	CH ₃ CH(Cl)COOC ₂ H ₅	136.58	2, 248	1.086_4^{20}	1.4185^{20}		147-148	38	i aq; misc alc, eth
	pionate									
e100	Ethyl 3-chloropro-	ClCH ₂ CH ₂ COOC ₂ H ₅	136.58	2, 250	1.1086_4^{20}	1.4249^{20}		163	54	misc alc, eth
	pionate									
e101	Ethyl chlorothio-	ClC(=O)SCH ₂ CH ₃	124.59	3, 134	1.195	1.4820^{20}		132	30	
	formate									
e102	Ethyl chrysanth-		196.29	$9^2, 45$	0.906	1.4600^{20}		112 ^{10mm}		
	emumate									

Ethyl benzyl ether, b95 Ethyl bromide, b277 Ethyl 2-bromo-2-methylpropanoate, e78 Ethyl bromopyruvate, e79 Ethyl bromovalerate, e80 Ethyl butyl ether, b449 Ethyl butyl ketone, h16 Ethyl caprate, e113 Ethyl caproate, e142 Ethyl caprylate, e190 Ethyl chloride, c102 Ethyl chloroglyoxylate, e191

$$CH_3$$
 $CH = C(CH_3)_2$
 CH_3
 $CH = C(CH_3)_2$
 CH_3
 $CH = C(CH_3)_2$
 $CH = C(CH_3)_2$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e103	Ethyl <i>trans</i> -cinnamate	C ₆ H ₅ CH=CHCOOCH ₂ CH ₃	176.22	9 ² , 385	1.0495420	1.559820	12	271.0		misc alc, eth; i aq
e104 e105 e106 e107	Ethyl crotonate Ethyl cyanoacetate Ethyl cyanoformate Ethyl cyano(hydroxy-	CH ₃ CH=CHCOOCH ₂ CH ₃ NCCH ₂ COOCH ₂ CH ₃ NCCOOCH ₂ CH ₃ NCC(=NOH)COOCH ₂ CH ₃	114.14 113.12 99.09 142.12	2, 411 2, 585 2, 547 3, 775	$ \begin{array}{c} 0.9175_4^{20} \\ 1.0564_4^{25} \\ 1.003_4^{20} \end{array} $	$ \begin{array}{r} 1.4248^{20} \\ 1.4156^{20} \\ 1.3820^{20} \end{array} $	-22.5 130-132	138 206.0 116	2 110 24	i aq; s alc, eth i aq; misc alc, eth
e108 e109	imino)acetate Ethylcyclohexane cis-2-Ethylcyclohexanol	C ₆ H ₁₁ CH ₂ CH ₃ CH ₃ CH ₂ C ₆ H ₁₀ OH	112.22 128.22	5, 35 6 ² , 26	$\begin{bmatrix} 0.7879^{20} \\ 0.927_4^{21} \end{bmatrix}$	1.4330 ²⁰ 1.4646 ²⁰	-111.3	131.8 74–79 ^{12mm}	18 68	i aq
e110 e112	4-Ethylcyclohexanol Ethyl cyclohexyl- acetate	CH ₃ CH ₂ C ₆ H ₁₀ OH C ₆ H ₁₁ CH ₂ COOCH ₂ CH ₃	128.22 170.25	6 ² , 26 9, 14	0.889 0.948	1.4625 ²⁰ 1.4439 ²⁰		84 ^{10mm} 212	77 80	
e112	Ethyl cyclopropane- carboxylate	C ₃ H ₅ COOCH ₂ CH ₃	114.14	9, 4	0.960	1.4197 ²⁰		129–133	18	
e113 e114	Ethyl decanoate Ethyl diazoacetate	CH ₃ (CH ₂) ₈ COOCH ₂ CH ₃ N ₂ CH ₂ COOCH ₂ CH ₃	200.32 114.10	2, 356 3 ¹ , 211	$0.862^{20} \\ 1.0852^{18}_{4}$	1.4248 ²⁰ 1.4588 ¹⁸	-22	245 141 ^{720mm} explodes	102 26 s when he	misc alc, chl, eth misc alc, bz, eth eated
e115	Ethyl 2,3-dibromopropionate	BrCH ₂ CH(Br)COO- CH ₂ CH ₃	259.94	2, 259	1.78846	1.4986 ²⁰		214	91	s alc, eth
e116	Ethyl dichloro- phosphate	CH ₃ CH ₂ OP(O)Cl ₂	162.94	1,332	1.373	1.433820		65 ^{10mm}		
e117	Ethyl dichloro- thiophosphate	CH ₃ CH ₂ OP(S)Cl ₂	179.01	1, 333	1.353	1.5040 ²⁰		55–68 ^{10mm}		
e118	N-Ethyldiethanol- amine	CH ₃ CH ₂ N(CH ₂ CH ₂ OH) ₂	133.19	4, 284	1.014	1.4665 ²⁰	-50	246–252	123	
e119	Ethyl diethoxy- phosphinylformate	$(C_2H_5O)_2P(O)COOC_2H_5$	210.17	3 ² , 103	1.110	1.4230 ²⁰		135 ^{13mm}		

e120	Ethyl 3-(diethyl-amino)propionate	(C ₂ H ₅) ₂ NCH ₂ CH ₂ - COOC ₃ H ₅	173.26	4, 404	0.881	1.4253^{20}		84 ^{12mm}	7	
e121	Ethyl 3,3-dimethyl- acrylate	$(CH_3)_2C = CHCOOC_2H_5$	128.17	2, 433	0.9247_4^{20}	1.4350^{20}		155	33	
e122	Ethyl 2-dimethyl- aminobenzoate	(CH ₃) ₂ NC ₆ H ₄ COOC ₂ H ₅	193.25		1.061	1.5425 ²⁰			98	
e123	Ethyl 2,2-dimethyl- propionate	(CH ₃) ₃ CCOOCH ₂ CH ₃	130.19	$2^2, 280$	0.8584_4^{18}	1.392218		118.2		s alc, eth
e124	Ethylene carbonate		88.06	19, 100	1.320825	1.4199^{40}	36.4	238	160	misc aq
e125	Ethylenediamine- N,N,N',N'-tetra- acetic acid	(HOOCCH ₂) ₂ NCH ₂ CH ₂ - N(CH ₂ COOH) ₂	292.24				245 d			0.05 aq
e126	Ethylene dinitrate	O2NOCH2CH2ONO2	152.07		1.496_{15}^{15}	1.499^{15}	-22	106 ^{19mm}		
e127	2,2'-(Ethylenedioxy)- bisethanol	HOCH ₂ CH ₂ OCH ₂ CH ₂ - OCH ₂ CH ₂ OH	150.17		1.127445	1.457815	-72	285	166	misc aq, alc, bz
e128	Ethylene glycol	HOCH ₂ CH ₂ OH	62.07	1, 465	1.1135 ₄ ²⁰	1.4319^{20}	-13	197.6	110	misc aq, alc, acet, glc, HOAc, pyr;
e129	Ethylene oxide	H_2C-CH_2	44.05		0.8914	1.35977	-112.44	10.6	-18	sl s eth; i bz, chl misc aq; s alc, eth
		U								

Ethyl 2-cyano-3-ethoxyacrylate, e132 *N*-Ethyldiisopropylamine, d418 Ethylene bromohydrin, b279 Ethylene chlorohydrin, c103 Ethylene cyanohydrin, h169 Ethylene diacetate, e17

Ethylenediamine, e15 Ethylene dibromide, d78 Ethylene dichloride, d177 (Ethylenedinitrilo)tetraacetic acid, e125 2,2'-Ethylenedioxybis (ethanol), t270 Ethylene glycol, e16 Ethylene glycol *p*-butylphenyl ethers, b475, b476
Ethylene glycol diacetate, e17
Ethylene glycol diethyl ether, d252
Ethylene glycol dimethyl ether, d439
Ethylene glycol dinitrate, e126

$$H_2C-O$$
 \downarrow
 H_2C-O
 $e124$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e130	Ethylene sulfide	H ₂ C-CH ₂	60.12	17 ² , 12	1.010	1.493520		55–56	10	sl s alc, eth
e131	Ethylenimine	H ₂ C-CH ₂ NH	43.07		0.8321425	1.4123 ²⁵	-78.0	56	-24	misc aq; sl s alc
e132	Ethyl (ethoxymethyl- ene)cyanoacetate	C ₂ H ₅ OCH=C(CN)- COOC ₂ H ₅	169.18	3,470			51–53	190 ^{30mm}		
e133	Ethyl fluoroacetate	FCH ₂ COOC ₂ H ₅	106.10	2, 193	1.092621	1.3755^{20}		119 ^{753mm}	30	s aq
e134	Ethyl fluoro- sulfonate	FSO ₂ OC ₂ H ₅	128.12					23- 25 ^{12mm}	32	
e135	Ethyl formate	HCOOC ₂ H ₅	74.08	2, 19	0.917_4^{20}	1.3599^{20}	-79.4	54.2	-28	12 aq; misc alc, eth
e136	Ethyl 2-furoate		140.14	18, 275	1.117_4^{20}		33–36	196	70	i aq; s alc, eth
e137	Ethyl heptafluoro- butyrate	CF ₃ CF ₂ CF ₂ COOC ₂ H ₅	242.09		1.394 ²⁰	1.3030^{20}		94–96		
e138	Ethyl heptanoate	CH ₃ (CH ₂) ₅ COOC ₂ H ₅	158.24	$2^2, 295$	0.8685_4^{20}	1.4144^{15}	-66	187		s alc, eth
e139	Ethyl hexadecanoate	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	284.48	$2^2,336$	0.8577_4^{25}	1.4347^{34}	22	191 ^{10mm}		s alc, eth
e140	3-Ethylhexane	CH ₃ CH ₂ CH ₂ CH(C ₂ H ₅) ₂	114.24	$1^3,478$	0.7136_4^{20}	1.4016^{20}		118.5		sl s alc; s eth
e141	2-Ethyl-1,3- hexanediol	C ₃ H ₇ CH(OH)CH- (C ₂ H ₅)CH ₂ OH	146.23		0.9325_4^{22}	1.4530^{22}	-40	244.2	129	0.6 aq; s alc
e142	Ethyl hexanoate	CH ₃ (CH ₂) ₄ COOC ₂ H ₅	144.21	2, 323	0.871_4^{20}	1.4075^{20}	-67	166-168	49	i aq; misc alc, eth
e143	2-Ethylhexanoic acid	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- COOH	144.21	2, 349	0.9077_{20}^{20}	1.424120	-118.4	227.6	127	0.25 aq
e144	2-Ethyl-1-hexanol	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ OH	130.23		0.9344_{20}^{20}	1.4231 ²⁰	-76	184.3	77	0.07 aq; s alc, bz,
e145	2-Ethylhexanoyl chloride	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- COCl	162.66	2^2 , 304	0.939	1.4335^{20}		68 ^{11mm}	69	
e146	2-Ethylhexyl acetate	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ OOCCH ₃	172.27		0.8718_{20}^{20}	1.4204 ²⁰	-93	198.6	82	0.03 aq; misc alc

e147	2-Ethylhexylamine	CH ₃ (CH ₂) ₃ CH(C ₂ H ₅)- CH ₂ NH ₂	129.31		0.792_{20}^{20}			165–169	57	i aq; s alc, acet,
		- 4 - 4			20					eth
e148	2-Ethylhexyl vinyl	$CH_3(CH_2)_3CH(C_2H_5)$ -	156.26		0.8102_{20}^{20}	1.4273^{20}	<100	177.7		0.01 aq
	ether	CH ₂ OCH=CH ₂					glass			
e149	Ethyl hydrogen	HOOC(CH ₂) ₄ COOC ₂ H ₅	174.20	21, 277		1.4387^{20}	28–29	180 ^{18mm}	>112	
01.7	hexanedioate	11000(0112)400002115	17.120	_ , _ , . ,		11.007	20 27	100	112	
e150	Ethyl hydroxyacetate	HOCH ₂ COOC ₂ H ₅	104.11	3, 236	1.087_4^{15}			160		v s alc, eth
e151	Ethyl 4-hydroxy-	HOC ₆ H ₄ COOC ₂ H ₅	166.18	10, 159			116	297 d		0.07 aq; v s alc, eth
	benzoate			,,						
-150		CH CH(OH)CH COOC H	122.16	2 200	1.0174	1.4205^{20}		170	64	1 .
e152	Ethyl 3-hydroxy- butyrate	CH ₃ CH(OH)CH ₂ COOC ₂ H ₅	132.16	3, 309	1.0174	1.4205		170	64	s aq, alc
e153	Ethyl 2-hydroxy-	HOCH ₂ CH ₂ SCH ₂ CH ₂	106.19	1 ² , 525	1.020_{20}^{20}	1.4869^{20}		184.5		s eth
	ethyl sulfide			- ,	20					
e154	Ethyl 2-hydroxy-	(CH ₃) ₂ C(OH)COOC ₂ H ₅	132.16	3, 315	0.965	1.4078^{20}		150	44	d hot aq
	isobutyrate									•
e155	Ethyl 4-hydroxy-3-	HOC ₆ H ₃ (OCH ₃)CH ₂ -	210.23	10 ¹ , 198			44-47	180-		
	methoxyphenyl-	COOC ₂ H ₅		· ·				185 ^{14mm}		
	acetate	20002115						100		
	acciaic			I	1		I	1	1	

Ethylene glycol monoacetate, h116 Ethylene glycol monobutyl ether, b410 Ethylene glycol monoethyl ether, e34 Ethylene glycol monomethyl ether, m65 Ethylene glycol monomethyl ether acetate, m68 Ethylene iodide, d403 Ethylene iodohydrin, i35 1,8-Ethylenenaphthalene, a2 Ethylenethiourea, i5 Ethylene trichloride, t227 Ethyleneurea, i7 *N*-Ethylethanamine, d267 Ethyl *N*-ethylcarbamate, e231 Ethylethylene oxide, e3

Ethyl fluroide, f17 2-Ethylhexyl alcohol, e144 Ethyl homovanillate, e155 *N*-Ethyl-*N*-(2-hydroxyethyl)-3-toluidine, e225 Ethyl 2-hydroxy-2-methylpropanoate, e154

$$C - OC_2H$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e156	2-Ethyl-2-(hydroxy- methyl)-1,3- propanediol	CH ₃ CH ₂ C(CH ₂ OH) ₃	134.18	13, 2349			60–62	159– 161 ^{2mm}		
e157	N-Ethyl-3-hydroxy- piperidine		129.20		0.970	1.4754 ²⁰		93– 95 ^{15mm}	47	
e158	5-Ethylidene-2- norbornene		120.20		0.893	1.4895			38	
e159	2-Ethylimidazole		96.13				79-81			
e160	2-Ethyl-6-isopropyl- aniline	(CH ₃) ₂ CHC ₆ H ₃ - (C ₂ H ₅)NH ₂	163.26		0.949			249		
e161	Ethyl isothiocyanate	CH ₃ CH ₂ NCS	87.14	4, 123	1.003_4^{18}	1.514218	-6	130-132	32	i aq; misc alc, eth
e162	Ethyl L-(+)-lactate	CH ₃ CH(OH)COOC ₂ H ₅	118.13	3, 264	1.032820	1.4124 ²⁰	-26	154.5	70	misc aq, alc, eth, esters, PE
e163	Ethyl DL-mandelate	C ₆ H ₅ CH(OH)COOC ₂ H ₅	180.21	10, 202			37	253–255		
e164	Ethyl 2-mercapto- acetate	HSCH ₂ COOC ₂ H ₅	120.17	3, 255	1.096415	1.4571 ²⁰		54 ^{12mm}	47	s alc, eth
e165	Ethylmercury chloride	CH ₃ CH ₂ HgCl	165.13		3.5		192	subl		0.78 eth; 2.6 chl
e166	Ethyl methacrylate	$H_2C = C(CH_3)COOC_2H_5$	114.14	2,423	0.909_{15}^{25}	1.4116^{25}		118	49	i aq; s alc, eth
e167	Ethyl 4-methoxy- phenylacetate	CH ₃ OC ₆ H ₄ CH ₂ COOC ₂ H ₅	194.23	10 ¹ , 83	1.097	1.5075 ²⁰		138 ^{7mm}	46	
e168	Ethyl 2-methylaceto- acetate	$CH_3C(=O)CH(CH_3)-COOC_2H_5$	144.17	3, 679	1.019_4^{20}	1.418220		187	62	i aq; s alc, eth
e169	N-Ethyl-N-methyl- aniline	$C_6H_5N(CH_3)C_2H_5$	135.21	12, 162	0.9193_4^{55}	1.5474 ²⁰		203–205		i aq; misc alc, eth
e170	Ethyl 3-methyl- butyrate	(CH ₃) ₂ CHCH ₂ COOC ₂ H ₅	130.19	$2^2, 275$	0.868^{20}_{20}	1.396220	-99.3	134.7	26	0.2 aq; misc alc, bz
e171	Ethyl methyl ether	CH ₃ CH ₂ OCH ₃	60.09	1, 314	0.725^{0}_{0}			10.8		s aq; misc alc, eth

e172	2-Ethyl-4-methyl- imidazole		110.16	$23^2,72$	0.975	1.4995^{20}		292–295	137	
e173	Ethyl 4-methyl-5- imidazolecarb-		154.17	25 ¹ , 534			204–206			
	oxylate									
e174	3-Ethyl-2-methyl-	$(C_2H_5)_2CHCH(CH_3)_2$	114.24	$1^3,489$	0.7193_4^{20}	1.4040^{20}	-115.0	115.7		i aq; sl s alc; s eth
	pentane									
e175	3-Ethyl-3-methyl-	$(C_2H_5)_3CCH_3$	114.24		0.7274_4^{20}	1.4078^{20}	-90.9	118.3		i aq; s eth
	pentane									
e176	Ethyl 3-methyl-3-		206.24		1.09_4^{15}	1.508^{20}				
	phenylglycidate									
e177	Ethyl 1-methyl-2-		171.24	22 ¹ , 485	0.975	1.4519^{20}		92-	73	
	piperidinecarb-							96 ^{11mm}		
	oxylate									

Ethyl 2-hydroxypropionate, e162 Ethylidene bromide, d77 Ethylidene chloride, d176 Ethylidene dimethyl ether, d438 Ethylidene fluoride, d346 2,2'-Ethyliminodiethanol, e118 Ethyl iodide, i34 Ethyl isonicotinate, e216 Ethyl isonipecotate, e206 Ethyl isopropylacetate, e170 Ethyl isothiocyanatoformate, e32 Ethyl isovalerate, e170 Ethyl levulinate, e195 Ethyl linoleate, e188

Ethyl mercaptan, e20
Ethyl 3-methylcrotonate, e121
Ethyl methyl ketone, b393
Ethyl 1-methylnipecotate, e177
Ethyl 2-methyl-4-oxo-2-cyclohexene-1-carboxylate, c9
Ethyl 1-methylpipecolinate, e178

OH
$$C_{2}H_{5}$$
 $C_{2}H_{5}$ $C_{2}H_{5}$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e178	Ethyl 1-methyl-3- piperidinecarb- oxylate		171.24		0.954	1.4510 ²⁰		89 ^{11mm}		
e179	2-Ethyl-2-methyl- 1,3-propanediol	HOCH ₂ C(C ₂ H ₅)(CH ₃)- CH ₂ OH	118.18	1,487			41–44	226		
e180	3-Ethyl-4-methyl- pyridine	$C_2H_5(CH_3)C_5H_3N$	121.18	20 ² , 163	0.9286_4^{17}			198		s alc, eth; sl s aq
e181	5-Ethyl-2-methyl- pyridine	$C_2H_5(CH_3)C_5H_3N$	121.18	20, 248	0.9184_4^{23}	1.4974 ²⁰		178	66	s alc, bz, eth, acid
e182	Ethyl methyl sulfide	CH ₃ CH ₂ SCH ₃	76.15	1, 343	0.842220	1.4403 ²⁰	-105.9	66.7	49	i aq; misc alc, eth
e183	Ethyl (methylthio)- acetate	CH ₃ SCH ₂ COOC ₂ H ₅	134.20		1.043	1.4587 ²⁰			59	
e184	N-Ethylmorpholine		115.18	271, 203	0.916_{20}^{20}	1.4410^{20}	-63	139	27	misc aq, alc, eth
e185	Ethyl nitrate	CH ₃ CH ₂ ONO ₂	91.13	1, 329	1.100_4^{25}	1.3849 ²²	-94.6	87.7	flam- mable	1 aq; misc alc, eth
e186	Ethyl nitrite	CH ₃ CH ₂ ONO	75.07	1, 329	0.90^{15}_{15}			17		misc alc, eth
e187	4-Ethylnitrobenzene	$C_2H_5C_6H_4NO_2$	151.17	5, 358	1.118	1.544520	-32	245-246	>112	v s alc, eth
e188	Ethyl (<i>Z</i> , <i>Z</i>)-9,12- octadecadienoic acid	H(CH ₂) ₅ CH=CHCH ₂ - CH=CH(CH ₂) ₇ COOC ₂ H ₅	308.51	2 ² , 461	0.884646	1.4675 ²⁰		193 ^{6mm}	>112	misc DMF, oils
e189	Ethyl cis-9-octa- decenoate	$CH_3(CH_2)_7CH = CH - (CH_2)_7COOC_2H_5$	310.52	2, 467	0.869_4^{20}	1.445 ²⁵	<-15	216 ^{15mm}		i aq; misc alc, eth
e190	Ethyl octanoate	CH ₃ (CH ₂) ₆ COOC ₂ H ₅	172.27	2, 348	0.878^{17}	1.4166^{20}	-47	206-208	75	i aq; misc alc, eth
e191	Ethyl oxalyl chloride	CH ₃ CH ₂ OC(=O)COC1	136.53	2, 541	1.2223420	1.4164 ²⁰		135	41	d aq, alc; s bz, eth
e192	Ethyl oxamate	$CH_3CH_2OC(=O)CONH_2$	117.10	2, 544			114–116			s aq, eth; i bz
e193	2-Ethyl-2-oxazoline		99.13		0.982	1.4370^{20}	-62	128.4	29	

e194	Ethyl 2-oxocyclo- pentanecarb-	$(O=)C_5H_7COOC_2H_5$	156.18		1.054	1.4485 ²⁰		102 ^{11mm}	>112	
	oxylate									
e195	Ethyl 4-oxopent-	$CH_3C(=O)CH_2CH_2$	144.17	3, 675	1.012_{20}^{20}	1.4222^{20}		205–206		v s aq; misc alc
	anoate	COOC ₂ H ₅								
e196	Ethyl 2-oxopropionate	$CH_3C(=O)COOC_2H_5$	116.12	3,616	1.060_4^{16}	1.40816		144	45	sl s aq; misc alc, eth
e197	3-Ethylpentane	(C ₂ H ₅) ₃ CH	100.20	$1^3,441$	0.6982_4^{20}	1.3934^{20}	-118.6	93.5		i aq; s alc, eth
e198	Ethyl pentanoate	CH ₃ (CH ₂) ₃ COOC ₂ H ₅	130.19	2, 301	0.877_4^{20}	1.3732^{20}	-91.3	145.5		0.2 aq; misc alc, eth
e199	4-Ethylphenol	CH ₃ CH ₂ C ₆ H ₄ OH	122.17	6, 472	1.011_4^{25}	1.5239	47.0	218-219		i aq; misc alc, eth
e200	Ethyl phenylacetate	C ₆ H ₅ CH ₇ COOC ₇ H ₅	164.20	9, 434	1.0333_4^{20}	1.4980^{20}		226	77	i aq; misc alc, eth
e201	Ethyl N-piperazino-		158.20	$23^2, 9$	1.080	1.4765^{20}		273	>112	
	carboxylate									
e202	1-Ethylpiperidine		113.20	20, 17	0.8237_4^{20}	1.4440^{20}		131	18	
e203	2-Ethylpiperidine		113.20	20, 104	0.850	1.4510^{20}		143	31	s aq
e204	Ethyl 2-piperidine-		157.21	22, 7	1.006	1.4562^{20}		216-217	46	_
	carboxylate									
e205	Ethyl 3-piperidine-		157.21		1.012	1.4601^{20}		104 ^{7mm}	90	
	carboxylate									

Ethyl nicotinate, e215 Ethyl nipecotate, e205 Ethyl oleate, e189 Ethyl pentyl ketone, o35 Ethyl phenyl ether, e28 Ethyl picolinate, e214

Ethyl pipecolinate, e204 Ethylpiperidinol, e157

$$C - OC_2H_5$$
 $C - OC_2H_5$
 $C - OC_2H_5$

$$\begin{array}{c}
H \\
N \\
O = C - OC_2H_5
\end{array}$$
e201

$$N$$
 C_2H_5
 C_2H_5

e203

e202

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e206	Ethyl 4-piperidine- carboxylate		157.21		1.010	1.459120		204	80	s aq, alc, bz, eth
e207	Ethyl <i>N</i> -piperidine- propionate		185.27	20, 62	0.927	1.4545 ²⁰		217–219	87	
e208	Ethyl propionate	CH ₃ CH ₂ COOC ₂ H ₅	102.13	2, 240	0.891_4^{20}	1.3839^{20}	-73.9	99.1	12	2 aq; misc alc, eth
e209	Ethyl propyl ether	CH ₃ CH ₂ OCH ₂ CH ₂ CH ₃	88.15	1, 354	0.739_4^{20}	1.3695^{20}	-79	62–63	32	sl s aq; misc alc, eth
e210	Ethyl propyl sulfide	CH ₃ CH ₂ SCH ₂ CH ₂ CH ₃	104.21	1^3 , 1432	0.8270_4^{20}	1.4462^{20}	-117.0	118.5		s alc
e211	2-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 241	0.937	1.4964^{20}		149	29	sl s aq; s alc, eth
e212	3-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 242	0.954	1.5015^{20}		162–165	48	v s alc, eth; sl s aq
e213	4-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 243	0.9404_4^{22}	1.5009^{20}		168	47	sl s aq; s alc, eth
e214	Ethyl 2-pyridine- carboxylate		151.17	22, 35	1.1194 ²⁰	1.5088^{20}	2	240–241	107	misc aq, alc, eth
e215	Ethyl 3-pyridine- carboxylate		151.17	22, 39	1.1070 ²⁰	1.5040^{20}	8–9	23–224	93	v s aq, alc, eth; s bz
e216	Ethyl 4-pyridine- carboxylate		151.17	$22^2, 37$	1.009_4^{15}	1.5009^{20}	23	220	87	i aq; s alc, bz, chl
e217	1-Ethyl-2-pyrrol-idinone		113.16		0.992	1.465220		97 ^{20mm}	76	
e218	Ethyl salicylate	C ₆ H ₄ (OH)COOC ₂ H ₅	166.18	10, 73	1.131_4^{20}	1.5219^{20}	2–3	231–234	107	misc alc, eth; sl s
e219	Ethyl sorbate	CH ₃ CH=CHCH=CH- COOC ₃ H ₅	140.18	2, 484	0.959	1.4942^{20}		195.5	69	
e220	S-Ethyl thioacetate	CH ₃ C(=O)SCH ₂ CH ₃	104.16	2, 232	0.976_4^{28}	1.4503^{28}		116–117		i aq; v s alc, eth
e221	3-Ethylthio-1,2- propanediol	C ₂ H ₅ SCH ₂ CH(OH)CH ₂ OH	136.21	_,	1.095	1.5065^{20}			>112	2
e222	Ethyl 4-toluene- sulfonate	CH ₃ C ₆ H ₄ SO ₂ OC ₂ H ₅	200.26	11,99	1.16645	1.5110^{20}	33	173 ^{15mm}	157	i aq; s alc, eth
e223	<i>N</i> -Ethyl- <i>m</i> -toluidine	CH ₃ C ₆ H ₄ NHC ₂ H ₅	135.21	12, 857	0.957	1.5451^{20}		221	89	

e224 e225	6-Ethyl- <i>o</i> -toluidine 2-(<i>N</i> -Ethyl- <i>m</i> - toluidino)ethanol	CH ₃ CH ₂ C ₆ H ₃ (CH ₃)NH ₂ CH ₃ C ₆ H ₄ N(C ₂ H ₅)CH ₂ - CH ₂ OH	135.21 179.26		0.968 1.019	$1.5525^{20} 1.5540^{20}$	-33	231 115 ^{1mm}	89	
e226	Ethyl trichloro- acetate	Cl ₃ CCOOC ₂ H ₅	191.44	2, 209	1.383420	1.4447 ²⁰		168	65	i aq; s alc, eth
e227	Ethyl trifluoro- acetate	F ₃ CCOOC ₂ H ₅	142.08	2 ² , 186	1.194	1.3068^{20}		60–62	-1	
e228	Ethyl (trimethyl-silyl)acetate	(CH ₃) ₃ SiCH ₂ COOC ₂ H ₅	160.29		0.876	1.4153^{20}		156–159	35	
e229	Ethyl undecanoate	CH ₃ (CH ₂) ₉ COOC ₂ H ₅	214.35	2,358	0.859	1.4280^{20}		105 ^{4mm}	>112	i aq; s org solv
e230	Ethylurea	$CH_3CH_2NHC(=O)NH_2$	88.11	4, 115	1.21318		93-96			v s aq; 80 alc; i eth
e231	<i>N</i> -Ethylurethane	CH ₃ CH ₂ NHCOOC ₂ H ₅	117.15	4, 114	0.981_4^{20}	1.4211^{20}		85 ^{20mm}	75	63 aq
e232	Ethyl vinyl ether	CH ₃ CH ₂ OCH=CH ₂	72.11	1,433	0.7531^{20}	1.3754^{20}	-115.8	35.7	-17	0.9 aq
e233	N-Ethyl-2,3- xylidine	$(CH_3)_2C_6H_3NHC_2H_5$	149.24	12, 1101	0.917	1.5468 ²⁰		227–228	71	•
e234	1-Ethynyl-1-cyclo- hexanol	C ₆ H ₁₀ (C≡CH)OH	124.18	6 ² , 100	0.967 ²⁰		30–31	180	62	2.4 aq; misc alc, bz, acet, ketones, PE

Ethyl pivalate, e123 1-Ethyl-1-propanol, p39 Ethyl propenoate, e56 1-Ethylpropylamine, a252 Ethyl pyruvate, e196 2-(Ethylthio)ethanol, e153 Ethyl thioglycolate, e164 Ethyltriethoxysilane, t261 Ethyl trimethylacetate, e123 Ethyl vanillin, e39 Ethyne, a41 Ethynylbenzene, p82

.25

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e235	1-Ethynylcyclo- hexylamine	$C_6H_{10}(C \equiv CH)NH_2$	123.30		0.913	1.481720		66 ^{20mm}	42	
f1 f2	Fluoranthene Fluorene		202.26 166.22	5, 685 5, 625	1.252 ₄ ⁰ 1.203 ₄ ⁰		107–110 114.8	384 295		sl s alc; s bz, eth v s HOAc; s bz, eth
f3 f4	9-Fluorenone Fluorescein		180.21 332.31	7, 465 19, 222	1.1300499	1.636999	82–85 314 d	342		s alc, bz; v s eth s hot alc, hot HOAc, alk; i bz, chl, eth
f5	Fluoroacetamide	FCH ₂ C(O)NH ₂	77.06	2, 193			107 subl			v s aq; s acet
f6 f7	Fluoroacetic acid Fluoroacetone	FCH ₂ COOH CH ₃ C(O)CH ₃ F	78.04 76.07	2, 193	1.054	1.3700	33	165 75	7	sl s aq, alc
f8	<i>p</i> -Fluoroaceto- phenone	FC ₆ H ₄ COCH ₃	138.14		1.138	1.5110^{20}		196	71	
f9	<i>p</i> -Fluoroaniline	FC ₆ H ₄ NH ₂	111.12	12, 597	1.1725_4^{20}	1.5395^{20}	-1.9	187	73	sl s aq; s alc, eth
f10	o-Fluorobenzal- dehyde	FC ₆ H ₄ CHO	124.11	7 ¹ , 132	1.178	1.5220 ²⁰	-44.5	91 ^{46mm}	55	
f11	Fluorobenzene	C ₆ H ₅ F	96.11	5, 198	1.0240_4^{20}	1.465720	-42.2	84.7	-12	0.15 aq; misc alc
f12	o-Fluorobenzoic acid	FC ₆ H ₄ COOH	140.11	9, 333	1.460_4^{25}		123–125			sl s aq; s alc, eth
f13	<i>p</i> -Fluorobenzoic acid	FC ₆ H ₄ COOH	140.11	9, 333	1.479_4^{25}		182.6			0.1 aq; s alc, eth
f14	<i>p</i> -Fluorobenzoyl chloride	FC ₆ H ₄ COCl	158.56	9 ¹ , 137	1.342	1.5296 ²⁰	9	82 ^{20mm}	82	
f15	o-Fluorobenzyl alcohol	FC ₆ H ₄ CH ₂ OH	126.13	6 ¹ , 222	1.173	1.5136 ²⁰			90	
f16	p-Fluorobenzyl chloride	FC ₆ H ₄ CH ₂ Cl	144.58		1.207	1.5130 ²⁰		82 ^{26mm}	60	
f17	Fluoroethane	CH ₃ CH ₂ F	48.06	1,82	0.002200		-143.2	-37.7		198 mL aq; v s alc, eth

f18	Fluoromethane	CH₃F	34.04	1,59	1.1951 g·L		-141.8	-78.4		166 mL aq; v s alc, eth
f19	4-Fluoro-1-methoxy- benzene	FC ₆ H ₄ OCH ₃	126.13	61,98	1.114	1.4877 ²⁰	-45	157	43	s eth
f20	2-Fluoro-2-methyl- propane	(CH ₃) ₃ CF	76.11	14, 286			-77	12.1	-12	
f21	1-Fluoro-4-nitro- benzene	FC ₆ H ₄ NO ₂	141.10	5, 241	1.3300_4^{20}	1.531220	21	205	83	i aq; s alc, eth
f22	4-Fluorophenol	FC ₆ H ₄ OH	112.10	6, 183			46-48	185	68	
f23	2-Fluoropyridine	FC ₅ H ₄ N	97.09	20 ¹ , 80	1.128	1.4680^{20}		126	28	
f24	o-Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	1.0014^{17}	1.4716^{17}	-62.0	114.4	12	v s alc, eth
f25	<i>m</i> -Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	0.9974^{20}	1.4691^{20}	-87.7	116.5	9	s alc, eth
f26	<i>p</i> -Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	0.9975^{20}	1.4688^{20}	-56.7	116.6	40	s alc, eth
f27	Formaldehyde	H ₂ C=O	30.03	1,558	0.815_4^{20}	0.8153^{-20}	-92	-19.5		122 aq; s alc, eth
f28	Formamide	$HC(=O)NH_2$	45.04	2, 26	1.1334_4^{20}	1.4475^{20}	2.6	111 ^{20mm}	154	misc aq, alc, acet
f29	Formamidine acetate	$HC(=NH)NH_2 \cdot HOOCCH_3$	104.11				158 d			_
f30	Formamidinesulfinic	$H_2NC(=NH)S(O)OH$	108.12	3 ¹ , 36			126 d			
	acid									

Eugenol, m99 Fenchone, t351 Fenchyl alcohol, t350 Ferulic acid, h136 2,7-Fluorenediamine, d38 *N*-9H-2-(2-Fluorenyl)acetamide, a13 Fluorotrichloromethane, t232 Fluothane, b258 Formic acid hydrazide, f34

f2

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
f31 f32 f33 f34	Formanilide Formic acid 2-Formylbenzoic acid Formylhydrazine	C ₆ H ₃ NHCHO HCOOH C ₆ H ₄ (HCO)COOH HC(=0)NHNH ₂	121.14 46.03 150.13 60.06	12, 230 2, 8 10, 666 2, 93	1.144 1.220 ₄ ²⁰ 1.404	1.3714 ²⁰	47 8.5 98 54–56	271 100.8	68	2.5 aq misc aq, alc, eth s aq; v s alc, eth v s alc, chl, eth; s bz
f35 f36	<i>N</i> -Formylpiperidine D-(-)-Fructose		113.16 180.16	20, 45 31, 321	1.019	1.4780 ²⁰		222	91	v s aq; 6.7 alc; s
f37	Fumaric acid	нооссн=снсоон	116.07	2,737	1.635 ₄ ²⁰		287	subl 200		0.6 aq; 9 alc; 0.7 eth
f38	Fumaroyl dichloride	CIC(=0)CH=CH- C(=0)Cl	152.96	2,743	1.408 ²⁰	1.4988 ²⁰		161–164	73	d aq, alc
f39	2-Furaldehyde		96.09	$17^2, 305$	1.1598_4^{20}	1.5262^{20}	-36.5	161.8	68	8 aq; misc alc, eth
f40	Furan		68.07	17, 27	0.9371_4^{20}	1.4214^{20}	-85.6	31.4	-35	1 aq; misc alc, eth
f41	2-Furanacrylic acid		138.12	18, 300			141	286		0.2 aq; 1.1 bz; s alc, eth, HOAc
f42	2-Furancarboxylic acid		112.08	18, 272			133–134	230–232		4 aq; s alc; v s eth
f43	2,5-Furandimethanol		128.13	17 ¹ , 90			74–76			
f44	2-Furanmethanethiol		114.17	$17^2, 116$	1.132	1.5304^{20}		155	45	
f45	Furfuryl acetate		140.14	$17^2, 115$	1.1175_4^{20}	1.4618^{20}		175–177	65	i aq; s alc, eth
f46	Furfuryl alcohol		98.10	17, 112	1.1285_4^{20}	1.4868^{20}	-14.6	170.0	65	misc aq(d); v s alc
f47	Furfurylamine		97.12	18, 584	1.0995_4^{20}	1.4900^{20}	-70	145–146	45	misc aq; s alc, eth
f48	2-Furoyl chloride		130.53	18, 276	1.324	1.5310^{20}	-2	170	85	d aq, alc; s eth
g1	D-(+)-Galactose		180.16	31, 295			167			200 aq; s pyr; sl s alc
g2	Geraniol	$(CH_3)_2C$ = $CHCH_2CH_2$ - $C(CH_3)$ = $CHCH_2OH$	154.25	1,457	0.8894_4^{20}	1.4760 ²⁰		230	76	i aq; misc alc, eth
g3	α -D-Glucoheptonic acid γ -lactone		208.17				145–148			s aq

Formylamide, f28 Formylphenols, h94, h95, h96 1-Formylpiperazine, p180 Formylpyridines, p251, p256, p253 Freon-11, t232 Freon-12, d170 Freon-12B2, d75 Freon-21, d183

Freon-22, c85

Freon-114, d227 2,5-Furandione, m2 2-Furanmethanol, f46 Furfural, f39 2-Furfuraldehyde, f39 Furfuryl mercaptan, f44 Furoic acid, f42 Furylacrylic acid, f41 2-Furyl methyl ketone, a44 Galactaric acid, t84 Galactitol, d738 Gallic acid, t306 Gallusic acid, t306 Gentisic acid, d384 Geranial, d562 D-Glucitol, s5

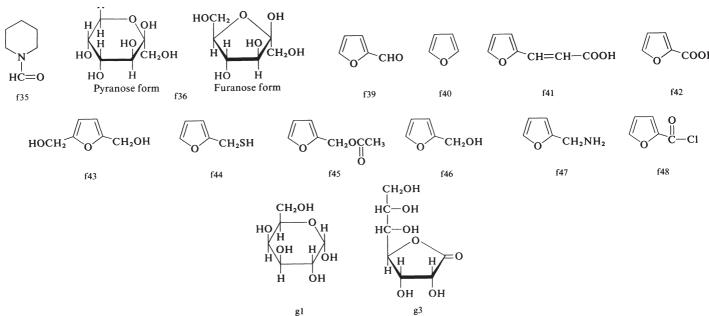


TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
g4 g5 g6	D-Gluconic acid D-Glucosamine α-D-(+)-Glucose		196.16 179.17 180.16	3, 542 1, 902 31, 83	1.562048		131 88(α) 146			v s aq; sl s alc; i eth v s aq; i chl, eth 91 aq; 0.83 MeOH; s pyr
g7	α-D-Glucose penta- acetate		390.34	31, 119			109–111			0.15 aq; 1.3 alc; 3 eth
g8	D-Glucurono-3,6- lactone		176.12				176–178			27 aq; 2.8 MeOH
g9	L-Glutamic acid		147.13	4, 488	1.538420		d 247	subl 200		0.8 aq; i alc, eth
g10	L-Glutamine		146.15	4, 491			d 185			4 aq; 0.0035 MeOH; i bz, chl, eth, acet
g11	Glutaric acid	HOOCCH ₂ CH ₂ CH ₂ COOH	132.12	2, 631	1.429_4^{20}	1.4188106	97.5	200 ^{20mm}		64 aq; v s alc, eth; s bz, chl; sl s PE
g12	Glutaric anhydride		114.10	17,411			52-55	150 ^{10mm}		, ,
g13	Glutaric dialdehyde	OCHCH ₂ CH ₂ CH ₂ CHO	100.12	1,776		1.3730^{20}	-6	187-189 d		misc aq, alc
g14	Glutaronitrile	NCCH ₂ CH ₂ CH ₂ CN	94.12	2, 635	0.9888^{23}	1.4345^{20}	-29	286	112	s aq, alc, chl; i eth
g15	Glutaryl dichloride	$ClC(=O)CH_2CH_2CH_2$ - $C(=O)Cl$	169.01	2, 634	1.324	1.4720 ²⁰		216–218	106	d aq, alc; s eth
g16	Glycerol	HOCH ₂ CH(OH)CH ₂ OH	92.09	1,502	1.2613 ²⁰	1.4746 ²⁰	18.18	182 ^{20mm}		misc aq, alc; 0.2 eth
g17	Glyceryl 1,2- diacetate	HOCH ₂ CH(OOCCH ₃)- CH ₂ OOCCH ₃	176.17	2, 147	1.1844	1.117315	40	172 ^{40mm}		s aq, alc, bz, eth
g18	Glyceryl 1,3- diacetate	CH ₃ COOCH ₂ CH(OH)- CH ₂ OOCCH ₃	176.17	2, 290	1.17915	1.4395 ²⁰	42	172 ^{40mm}		s aq, alc, bz, chl
g19	Glyceryl tris- (butyrate)	,	302.37	2, 273	1.032_4^{20}	1.4359 ²⁰	-75	305–310	173	i aq; v s alc, eth
g20	Glyceryl tris- (dodecanoate)		639.02	2, 363	0.894460	1.440460	46			v s bz, eth; sl s alc
	I	I	I	I	I	I	I	I	I	I

g21 g22 g23 g24	Glyceryl tris- (nitrate) Glyceryl tris- (oleate) Glyceryl tris- (palmitate) Glyceryl tris- (tetradecanoate)	O ₂ NOCH ₂ CH(ONO ₂)- CH ₂ ONO ₂	227.09 885.46 807.35 723.18	1,516 4,468 2,373 2,367	$ \begin{vmatrix} 1.594_4^{20} \\ 0.915_4^{15} \\ 0.8663_4^{80} \\ 0.885_4^{60} \end{vmatrix} $	1.4786 ¹² 1.4621 ⁴⁰ 1.4381 ⁸⁰ 1.4428 ⁶⁰	13.3 -4 to -5 65-66 57	160 ^{5mm} 235 ^{15mm} 310–320	expl 270	0.18 aq; 54 alc; misc eth s chl, eth, CCl ₄ v s bz, chl, eth v s alc, bz, chl
Glycera	aldehyde, g13 aldehyde, d398 ol dichlorohydrin, d220	Gl	ycerol α-mor yceryl triacet yceryl tris(lat	ate, p201	lrin, c212		Glyceryl t	ris(myristat	e), g24	
НОС	Н Н ОН Н Н2-С-С-С-С-СС НО ОН Н ОН g4	OOH CH ₂ OH OOH OOH HO OH HO NH ₂	H	он н	H CI	H	ОССН₃ Н	3 H OOCCH3	но	OCH O OH OH
	Н	H ₂ HC-NH ₂ CH ₂ CH ₂	$H_2)_8H$	CH ₂ − HC−O	g19	COC_3H_7 C_3H_7 COC_3H_7 COC_3H_7	CH ₂ -O HC-O-0	g20	27	
		g22	~-*2/8**	C11 ₂	g23	15**31	-	g24	21	

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
g25	Glycine	H ₂ NCH ₂ COOH	75.07	4, 333	1.1607		d 233			25 aq; 0.6 pyr; i
g26	N-Glycylglycine	H ₂ NCH ₂ C(=O)NHCH ₂ - COOH	132.12	4, 371			d 262			s hot aq; sl s alc
g27	Glyoxal	HC(=O)CHO	58.04	1,759	1.29420	1.3826 ²⁰	15	51		violent reaction aq; s anhyd solv; mixtures with air may explode
g28	Glyoxylic acid	HC(=O)COOH	74.04	3, 594			98			v s aq; sl s alc, eth
g29	Guanidine	$H_2NC(=NH)NH_2$	59.07	3, 82	0. == <=??	1 12 5025	~60	d 160	1.40	v s aq, alc
h1	Heptadecane	CH ₃ (CH ₂) ₁₅ CH ₃	140.41	1, 173	0.7767 ²²	1.4360^{25}	22.0	302.2	148	s eth; sl s alc
h2	Heptafluorobutyric acid	CF ₃ CF ₂ CF ₂ COOH	214.04		1.645			120		
h3	Heptafluoro-2,3,3- trichlorobutane	CF ₃ CCl ₂ CF(Cl)CF ₃	287.5		1.748420	1.3530 ²⁰	4	98		
h4	2,2,4,4,6,8,8-Hepta- methylnonane	(CH ₃) ₃ CCH ₂ C(CH ₃) ₂ CH ₂ - CH(CH ₃)CH ₂ C(CH ₃) ₃	226.45		0.793	1.4391 ²⁰		240		
h5	Heptanal	CH ₃ (CH ₂) ₅ CHO	114.19	1 ² , 750	0.8216_4^{15}	1.428520	-43	153	35	misc alc, eth; sl s
h6	Heptane	CH ₃ (CH ₂) ₅ CH ₃	100.21	1.154	0.6838_4^{20}	1.3877 ²⁰	-90.6	98.4	-1	s alc, chl, eth
h7	1,7-Heptanediamine	H ₂ N(CH ₂) ₇ NH ₂	130.24	4, 271	0.00004		27–29	147–149	87	
h8	Heptanedioic acid	HOOC(CH ₂) ₅ COOH	160.17	2,670	1.32915		105.8	212 ^{10mm}		5 aq; v s alc, eth
h9	1-Heptanethiol	CH ₃ (CH ₂) ₆ SH	132.27	1,415			-43.2	176.9	46	i aq
h10	Heptanoic acid	CH ₃ (CH ₂) ₅ COOH	130.19	2, 338	0.9181_4^{20}	1.422120	-7.5	223.0	>112	0.25 ag; s alc, eth
h11	Heptanoic anhydride	[CH ₃ (CH ₂) ₅ CO] ₂ O	242.36	2,340	0.932_4^{20}	1.4332^{20}	-12.4	268	>112	i aq; s alc, eth
h12	1-Heptanol	CH ₃ (CH ₂) ₆ OH	116.20	1,414	0.8219_4^{20}	1.4242^{20}	-34.6	175.8	73	misc alc, eth
h13	2-Heptanol	CH ₃ (CH ₂) ₄ CH(OH)CH ₃	116.20	1,415	0.8193_4^{70}	1.4210^{20}		160	41	0.35 aq; s alc, bz,
										eth

h14	3-Heptanol	CH ₃ (CH ₂) ₃ CH(OH)- CH ₂ CH ₃	116.20	11, 205	0.818	1.4214^{20}		66 ^{20mm}	54	sl s aq
h15	2-Heptanone	CH ₃ (CH ₂) ₄ COCH ₃	114.19	1,699	0.8197_4^{15}	1.411615	-35	151	47	s alc, eth
h16	3-Heptanone	$CH_3(CH_2)_3C(=O)$ -	114.19	1,699	0.8197_{20}^{20}	1.4085^{20}	-36.7	147.8	41	0.43 aq; s alc, eth
		CH ₂ CH ₃			15					
h17	4-Heptanone	CH ₃ CH ₂ CH ₂ (O)CH ₂ -	114.19	1,699	0.821_4^{15}	1.4068^{20}	-32.1	143.7	48	0.53 aq; misc alc,
		CH ₂ CH ₃								eth
h18	Heptanoyl chloride	CH ₃ (CH ₂) ₅ COCl	148.63	2,340	0.960^{20}	1.4300^{20}		173	57	d aq, alc; s eth
h19	1-Heptene	$CH_3(CH_2)_4CH = CH_2$	98.90	1,219	0.6970^{20}	1.3999^{20}	-118.9	93.6	-1	0.1 aq; s alc, eth
h20	1-Heptylamine	CH ₃ (CH ₂) ₆ NH ₂	115.22	4, 193	0.777	1.4243^{20}	-23	154-156	35	s alc, acet, eth, PE
h21	Heptyltrichlorosilane	CH ₃ (CH ₂) ₆ SiCl ₃	233.7		1.087_4^{20}	1.4439^{25}		211-212		
h22	1-Heptyne	CH ₃ (CH ₂) ₄ C≡CH	96.17	1, 256	0.733	1.4075^{20}	-81	99-100	22	
h23	Hexachloroacetone	Cl ₃ CC(=O)CCl ₃	264.75	1,657	1.743	1.5112^{20}	-30	66 ^{6mm}	none	sl s aq; s acet
h24	Hexachlorobenzene	C ₆ Cl ₆	284.78	5, 205	2.044^{24}		231	323-326		s bz, chl, eth
h25	Hexachloro-1,3-	Cl ₂ C=CClCCl=CCl ₂	260.76	1, 250	1.655	1.5550^{20}	-19	210-220	none	s alc, eth
	butadiene									
h26	1,2,3,4,5,6-Hexa-	C ₆ H ₆ Cl ₆	290.83	5^2 , 11	1.87^{20}		113			s bz, chl
	chlorocyclohexane									
h27	Hexachlorocyclo-1,3-		272.77		1.701_4^{25}	1.5644^{20}	-10	239	none	
	pentadiene									
	1	I .	I	1	1	1		1	1	I

Glycidol, e11 Glycidyl methacrylate, e12 Glycinonitrile, a106 Glycolaldehyde, h86 Glycolaldehyde diethyl acetal, d253 Glycolic acid, h87 Glycol methacrylate, h121 Glyoxaline, 14 Guaiacol, m87 Heliotropin, m239 Heliotropyl alcohol, m242 Hemimellitene, t333 Hemimellitic acid, b28 Heptaldehyde, h5

sec-Heptyl alcohol, h13 Heptyl bromide, b291 Heptyl chloride, c128 Heptyl iodide, i37 Heptyl mercaptan, h9 Hexachloro-2-propanone, h23

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h28 h29 h30	Hexachlorodisiloxane Hexachloroethane 1,4,5,6,7,7-Hexa- chloro-5-norborn-	Cl ₃ SiOSiCl ₃ Cl ₃ CCCl ₃	284.9 236.74 370.83	1, 87	2.091420		-35 187-188 235-239	137		s alc, bz, chl, eth
	ene-2,3-dicarbox- ylic anhydride									
h31	Hexachloropropene	$Cl_3CC(Cl) = CCl_2$	248.75	1, 200	1.765	1.5480^{20}		210	none	
h32	Hexadecane	CH ₃ (CH ₂) ₁₄ CH ₃	226.45	1, 172	0.7733_4^{20}	1.4345^{20}	18.2	286.8	135	misc eth
h33	1,2-Hexadecanediol	CH ₃ (CH ₂) ₁₃ CH(OH)- CH ₂ OH	258.45	1 ³ , 2244			72–74			
h34	1-Hexadecanethiol	CH ₃ (CH ₂) ₁₅ SH	258.51	1,430	0.840	1.4720^{20}	18-20	184 ^{7mm}	101	sl s alc; s eth
h35	Hexadecanoic acid	CH ₃ (CH ₂) ₁₄ COOH	256.43	2, 370	0.852_4^{62}	1.4273^{80}	63-64	215 ^{15mm}		s hot alc, chl, eth
h36	1-Hexadecanol	CH ₃ (CH ₂) ₁₅ OH	242.45	1, 429	0.811660	1.4355^{60}	49.3	344	135	s alc, chl, eth
h37	1-Hexadecene	$CH_3(CH_2)_{13}CH = CH_2$	224.43	1, 226	0.783_4^{20}	1.4401	4.1	274	132	s alc, eth, PE
h38	1-Hexadecylamine	CH ₃ (CH ₂) ₁₅ NH ₂	241.46	4, 202			40–42	330	140	v s alc, eth; s bz, chl
h39	4-Hexadecylaniline	CH ₃ (CH ₂) ₁₅ C ₆ H ₄ NH ₂	317.56	12, 1186			51–52	254– 255 ^{15mm}		
h40	2,4-Hexadienal	CH3CH=CHCH=CHCHO	96.13	$1^2,809$	0.898^{20}	1.5386^{20}		76 ^{30mm}	67	
h41	1,5-Hexadiene	H ₂ C=CHCH ₂ CH ₂ CH=CH ₂	82.15	1, 253	0.6923_4^{20}	1.4042^{20}	-140.7	59.5	<1	s alc, eth
h42	2,4-Hexadienoic acid	CH ₃ CH=CHCH= CHCOOH	112.13	2, 483			134.5	119 ^{10mm}	127	0.2 aq; 13 alc; 9 acet; 2.3 bz; 11 diox; 1 CCl ₄
h43	Hexafluorobenzene	C ₆ F ₆	186.05		1.6182^{20}	1.3781^{20}	5.1	80.3	10	
h44	Hexafluoroethane	F ₃ CCF ₃	138.01	$1^3, 132$	1.590^{-78}		-100.1	-78.3		sl s alc, eth
h45	1,1,1,3,3,3-Hexa- fluoro-2-propanol	(CF ₃) ₂ CHOH	168.04		1.596 ²⁵	1.2750^{20}	-3	58.2	4	s aq, bz, CCl ₄
h46	cis-Hexahydroindane		124.23	5, 82	0.876	1.4702	-53	167	23	s eth
h47	Hexamethylbenzene	C ₆ (CH ₃) ₆	162.28	5, 450			165.6	264		v s bz; s acet, eth

h48	Hexamethylcyclotri- siloxane	[—Si(CH ₃) ₂ O—] ₃	222.48	4^3 , 1884			64	133–135	35	
h49	1,1,1,3,3,3-Hexa- methyldisilazane	(CH ₃) ₃ SiNHSi(CH ₃) ₃	161.40		0.774_4^{20}	1.4071 ²⁰		126	22	
h50	Hexamethyldi- siloxane	(CH ₃) ₃ SiOSi(CH ₃) ₃	162.38		0.764_4^{20}	1.3775 ²⁰	-67	101	-1	
h51	Hexamethyleneimine		99.18	20, 94	0.880	1.4631^{20}		138 ^{749mm}	18	
h52	Hexamethylene- tetramine		140.19	1,583	1.331 ⁻⁵	subl 263			250	67 aq; 8 alc; 10 chl
h53	Hexamethylphosphor- amide	[(CH ₃) ₂ N] ₃ P(O)	179.20		1.027 ²⁰	1.4588 ²⁰	7.2	233	105	misc aq
h54	Hexanal	CH ₃ (CH ₂) ₄ CHO	100.16	1 ² , 745	0.8335_4^{20}	1.4035^{20}		131	32	v s alc, eth; sl s aq
h55	Hexane	CH ₃ (CH ₂) ₄ CH ₃	86.18	1, 142	0.6594_4^{20}	1.3749^{20}	-95.4	68.7	-23	misc alc, chl, eth
h56	1,6-Hexanediamine	$H_2N(CH_2)_6NH_2$	116.21	4, 269			42	205	81	v s aq; sl s alc, bz
h57	1,6-Hexanedioic acid	HOOC(CH ₂) ₄ COOH	146.14	2, 649	1.360425		152	337.5	196	1.4 aq; v s alc; s acet

 $\alpha,\alpha,\alpha,\alpha',\alpha',\alpha'$ -Hexachloro-p-xylene, b202 Hexadecyl mercaptan, h34 $\alpha,\alpha,\alpha,\alpha',\alpha',\alpha'$ -Hexafluoro-3,5-xylidine, b205 Hexahydroaniline, c334 Hexahydro-2H-azepin-2-one, o57 Hexahydrobenzaldehyde, c315 Hexahydrobenzoic acid, c317 Hexahydrobenzylamine, c324 Hexahydrophthalic acid, c320 Hexahydropyridine, p183 Hexamethylenediamine, h56 Hexamethylene diisocyanate, d410 Hexamethylene, glycol, h59 Hexamethylene oxide, o47 Hexamethylethane, t100 2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22tetracosahexene, s8 2,6,10,15,19,23-Hexamethyltetracosane, s7

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h58 h59	DL-Hexanediol 1,6-Hexanediol	CH ₃ (CH ₂) ₃ CH(OH)CH ₂ OH HO(CH ₂) ₆ OH	118.18 118.18	1 ¹ , 251 1, 484	0.951 0.958	1.4425 ²⁰ 1.4579 ²⁵	42.8	223–234 243–250	>112 101	v s aq, alc
h60	2,5-Hexanediol	CH ₃ CH(OH)CH ₂ CH ₂ - CH(OH)CH ₃	118.18	1,485	0.9617_{16}^{45}	1.4465 ²⁰	-50 glass	220.8	101	s aq, alc, eth
h61	2,5-Hexanedione	CH ₃ COCH ₂ CH ₂ COCH ₃	114.14	1,788	0.973	1.4260^{20}	-6	191.4	70	misc aq, alc, eth
h62	Hexanedioyl dichloride	$ClC(=O)(CH_2)_4COC1$	183.03	2, 653	1.259	1.4706 ²⁰		105 ^{2mm}	>112	
h63	Hexanenitrile	CH ₃ (CH ₂) ₄ CN	97.16	2, 324	0.8052^{20}	1.4069^{20}	-80.3	163.6	43	i aq; s alc, eth
h64	1-Hexanethiol	CH ₃ (CH ₂) ₅ SH	118.24	1 ³ , 1659	0.8424_4^{20}	1.4496^{20}	-80.5	152.7	20	i aq; v s alc, eth
h65	1,2,6-Hexanetriol	HOCH ₂ CH(OH)(CH ₂) ₃ - CH ₂ OH	134.17		1.1063_{20}^{20}	1.4771	-32.8	178 ^{5mm}	79	misc alc, acet; i bz
h66	Hexanoic acid	CH ₃ (CH ₂) ₄ COOH	116.16	2, 321	0.9265_4^{20}	1.4168^{20}	-4.0	205.7	104	1.1 aq; v s alc, eth
h67	Hexanoic anhydride	$[CH_3(CH_2)_4C(=O)]_2O$	214.31	2, 324	0.926	1.4280^{20}	-41	246-248	>112	s alc
h68	1-Hexanol	CH ₃ (CH ₂) ₅ OH	102.18	1, 407	0.8186_4^{20}	1.418220	-51.6	157.5	60	8 aq; misc bz, eth; s alc
h69	2-Hexanol	CH ₃ (CH ₂) ₃ CH(OH)CH ₃	102.18	1,408	0.8108_4^{25}	1.412825	-47	139.9	41	sl s aq; s alc, eth
h70	3-Hexanol	CH ₃ CH ₂ CH ₂ CH(OH)- CH ₂ CH ₃	102.18	1,408	0.8193_4^{20}	1.4160^{20}		135	41	_
h71	6-Hexanolactone		114.14	$17^2, 290$	1.030	1.4630^{20}		97 ^{15mm}	109	
h72	2-Hexanone	CH ₃ (CH ₂) ₃ COCH ₃	100.16	1,689	0.8209_4^{20}	1.4024^{20}	-56.9	127.2	35	v s alc, eth
h73	Hexanoyl chloride	CH ₃ (CH ₂) ₄ COCl	134.61	2, 324	0.9754_4^{20}	1.426320	-87	153	79	d aq, alc; s eth
h74	1,4,7,10,13,16-Hexa- oxacycloocta- decane		264.32				40			
h75	1-Hexene	CH ₃ (CH ₂) ₃ CH=CH ₂	84.16	1, 215	0.6732^{20}	1.387920	-139.8	63.5	-26	0.005 ag
h76	trans-3-Hexenoic	CH ₃ CH ₂ CH=CHCH ₂ -	114.14	2, 435	0.963	1.439820	11–12	119 ^{22mm}	>112	0.003 aq
1170	acid	COOH	** ' '	_, 133	0.703	1.1570	11.12	***	112	
h77	trans-2-Hexen-1-ol	CH ₃ CH ₂ CH ₂ CH=CH- CH ₂ OH	100.16	1 ² , 486	0.849	1.4343 ²⁰		158–160	54	

h78 h79 h80	5-Hexen-2-one Hexyl acetate Hexylamine	H ₂ C=CHCH ₂ CH ₂ COCH ₃ CH ₃ (CH ₂) ₅ OOCCH ₃ CH ₃ (CH ₂) ₅ NH ₂	98.15 144.21 101.19	1,734 2,132 4,188	$ \begin{vmatrix} 0.847 \\ 0.860_{20}^{20} \\ 0.763_{4}^{25} \end{vmatrix} $	$ \begin{array}{c} 1.4197^{20} \\ 1.4090^{20} \\ 1.4180^{20} \end{array} $	-80 -23	128–129 168–170 131–132	23 37 8	0.13 aq; v s alc, eth sl s aq; misc alc, eth
h81	4-Hexylaniline	CH ₃ (CH ₂) ₅ C ₆ H ₄ NH ₂	177.29	12 ³ , 2759				146– 148 ^{17mm}		Cui
h82 h83 h84 h85	1-Hexyne L-Histidine Hydantoin Hydrindantin	H(CH ₂) ₄ C≡CH	82.14 155.16 100.08 322.27	1 ³ , 977 25, 513 24, 242 8 ¹ , 631	0.71524	1.3989 ²⁰	-131.9 d 285 220 100	71.3 d 252		i aq; s alc, eth 41 aq; v sl s alc s alc, alk; sl s eth v sl s aq
h86 h87	Hydroxyacetaldehyde Hydroxyacetic acid	HOCH₂CHO HOCH₊COOH	60.05 76.05	1,817	1.366100		93–94 80	110 ^{12mm}		v s aq, alc; sl s eth

D-erythro-Hex-2-enoic acid γ -lactone, 159

Hexyl alcohol, h68 sec-Hexyl alcohol, e83 sec-Hexylamine, m353a Hexylbenzene, p117 Hexyl bromide, b294 Hexyl chloride, c129 Hexylene glycol, m338 Hexyl iodide, i39

Hexyl methyl ketone, o34 Hexyl propyl ketone, d16 Hippuric acid, b71 Histamine, i8 Homocysteine, a204 Homopiperidine, h51 Homoserines, a188, a189 Homoveratric acid, d447 Homoveratrylamine, d451

Hydracrylonitrile, h169 2-Hydrazinoethanol, h120 Hydrazobenzene, d673 Hydrindene, i13 Hydrocinnamic acid, p146 Hydroquinone, d379 Hydroquinone dimethyl ether, d433 Hydroquinonesulfonic acid, d382 Hydroxyacetanilides, a15, a16, a17

$$\begin{array}{c} & & H \\ N \\ N \\ \downarrow \\ HOOCCCH_2 \\ \downarrow \\ H \end{array}$$

h83

h84

h85

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h88	1'-Hydroxy-2'-aceto- naphthone	C ₁₀ H ₆ (OH)COCH ₃	186.21	8, 149			98–100	325 sl d		i aq; v s bz; s HOAc
h89	Hydroxyacetone	HOCH ₂ COCH ₃	74.08	11,84	1.082	1.4315^{20}	-17	145-146	56	misc aq, alc, eth
h90	o-Hydroxyaceto- phenone	HOC ₆ H ₄ COCH ₃	136.15	8, 85	1.13141	1.5584 ²⁰	4–6	213 ^{717mm}	>112	misc alc, eth; sl s
h91	<i>m</i> -Hydroxyaceto- phenone	HOC ₆ H ₄ COCH ₃	136.15	8, 86	1.100100	1.535100	87–88	296		s aq; v s alc, bz, eth
h92	<i>p</i> -Hydroxyaceto- phenone	HOC ₆ H ₄ COCH ₃	136.15	8, 87	1.109100		106–107	147 ^{3mm}		v s alc, eth; sl s aq
h93	1-Hydroxyanthra- quinone		224.22	8, 338			196–198			
h94	2-Hydroxybenz- aldehyde	C ₆ H ₄ (OH)CHO	122.12	8, 31	1.167_4^{20}	1.5718 ²⁰	-7	196.7	76	1.7 aq ⁸⁶ ; s alc, eth
h95	3-Hydroxybenz- aldehyde	C ₆ H ₄ (OH)CHO	122.12	8, 58			100–102	191 ^{50mm}		s alc, bz, eth; sl s
h96	4-Hydroxybenz- aldehyde	HOC ₆ H ₄ CHO	122.12	8, 64	1.129 ₄ ¹³⁰		117–119	subl		1 aq; 70 acet; 4 bz; v s alc, eth
h97	2-Hydroxybenz- aldehyde oxime	C ₆ H ₄ (OH)CH=NOH	137.14	8, 49			57	d		v s alc, bz, eth, acid
h98	2-Hydroxybenzamide	C ₆ H ₄ (OH)CONH ₂	137.14	10, 87			140	d 270		0.2 aq; s alc, chl, eth
h99	2-Hydroxybenzoic acid	C ₆ H ₄ (OH)COOH	138.12	10, 43	1.443 ²⁰		157–159	211 ^{20mm}		0.2 aq; 37 alc; 33 eth; 33 acet; 2 chl; 0.7 bz
h100	3-Hydroxybenzoic acid	C ₆ H ₄ (OH)COOH	138.12	10, 134	1.473		201–203			0.8 aq; 10 eth
h101	4-Hydroxybenzoic acid	HOC ₆ H ₄ COOH	138.12	10, 149	1.4684		214–215			0.2 aq; v s alc; 23 eth

h102	p-Hydroxybenzo-	HOC ₆ H ₄ COC ₆ H ₅	198.22	8 ² , 184			132–135			v s alc, eth; sl s aq
	phenone									
h103	1-Hydroxybenzo-		135.13	26, 41			155–158			
	triazole									
h104	6-Hydroxy-1,3-benz- oxathiol-2-one		168.17	19 ⁴ , 2508			158–160			
h105	2-Hydroxybenzyl alcohol	HOC ₆ H ₄ CH ₂ OH	124.13	6, 891	1.161 ²⁵		86–87	subl 100		6.6 aq; v s alc, chl, eth; s bz
h106	3-Hydroxy-2-buta-	CH ₃ COCH(OH)CH ₃	88.10	1,827	0.997	1.4171^{20}	15	148	50	misc aq, alc; sl s
	none									eth
h107	<i>p</i> -Hydroxycinnamic	$HOC_6H_4CH = CHCOOH$	164.16	10, 297			210–213			s alc, eth; sl s aq
	acid									
h108	4-Hydroxycoumarin		162.14	17, 488			213 d			s aq, alc, eth
h109	7-Hydroxycoumarin		162.14	18, 27			226–228	subl		v s alc, chl, alk,
										HOAc
h110	1-Hydroxy-1-cyclo- hexanecarbonitrile	$C_6H_{10}(OH)CN$	125.17	10, 5	1.031	1.4576^{20}	29		60	
h111	2-Hydroxy-3,5-	I ₂ C ₆ H ₂ (OH)COOH	389.91	10, 113			235 d			v s alc, eth; i bz,
	diiodobenzoic acid									chl
h112	2'-Hydroxy-4',6'-di-	(CH3)2C6H2(OH)-	164.20				53–57			
	methylaceto-	COCH ₃								
	phenone									

2-Hydroxybenzenemethanol, h105 *m*-Hydroxybenzotrifluoride, t290

2-Hydroxybiphenyl, p131 4-Hydroxybiphenyl, p132 Hydroxybutanedioic acids, h180, h181

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h113	2-Hydroxydiphenyl-	C ₆ H ₅ CH ₂ C ₆ H ₄ OH	184.24	6, 675			20.6	312		s alc, chl, eth, alk
h114	methane 2-Hydroxyethane- sulfonic acid, Na salt	HOCH ₂ CH ₂ SO ₃ Na ⁺	148.11	4 ³ , 42			191–194			v s aq
h115	N-(2-Hydroxyethyl)- acetamide	HOCH ₂ CH ₂ NHCOCH ₃	103.12	41, 430	1.123320	1.4575 ²⁰	63–65	d	176	misc aq: sl s bz
h116	2-Hydroxyethyl acetate	CH ₃ COOCH ₂ CH ₂ OH	104.11	2, 141	1.10815			181–186	102	misc aq, alc, chl,
h117	3-(α-Hydroxyethyl)- aniline	CH ₃ CH(OH)C ₆ H ₄ NH ₂	137.18	13 ³ , 1654			68–71			
h118	2-Hydroxyethyl disulfide	HOCH ₂ CH ₂ SSCH ₂ CH ₂ OH	154.25	1,471	1.261	1.5655 ²⁰	25–27	158 ^{3.5mm}		
h119	N-(2-Hydroxyethyl)- ethylenediamine- N,N,N'-triacetic acid	HOOCCH ₂ N(CH ₂ CH ₂ OH)- CH ₂ CH ₂ N(CH ₂ COOH) ₂	278.26				212 d			
h120	2-Hydroxyethyl- hydrazine	HOCH ₂ CH ₂ NHNH ₂	76.10	41,562	1.119		-70	220	73	misc aq; s alc
h121	2-Hydroxyethyl methacrylate	HOCH ₂ CH ₂ OOC- C(CH ₃)==CH ₂	130.14		1.034	1.4515 ²⁰		67 ^{3.5mm}	97	
h122	N-(β-Hydroxyethyl)- morpholine	3, - 2	131.18	27,7	1.083	1.4760 ²⁰		227	99	misc aq
h123	N-(β-Hydroxyethyl)- piperazine		130.19	23 ² , 6	1.061	1.5065 ²⁰		246	>112	
h124	N-(2-Hydroxyethyl)- piperazine-N'- ethanesulfonic acid		238.31				234 d			

h125	4'-(2-Hydroxyethyl)-		129.20	$21^2, 10$	1.0059_4^{15}			199–202		
	piperidine									
h126	2'-(2-Hydroxyethyl)-	HOCH ₂ CH ₂ C ₅ H ₄ N	123.16	21, 50	1.093	1.5368^{20}		116 ^{9mm}	92	v s aq, alc, chl
	pyridine									
h127	2-Hydroxyisobutyric	(CH ₃) ₂ C(OH)COOH	104.11	3,313			77-80	84 ^{1.5mm}		v s aq, alc, eth
	acid									
h128	4-Hydroxy-2-mer-		142.18	24 ³ , 1289			330 d			
	capto-6-methyl-									
	pyrimidine									
h129	4-Hydroxy-2-mer-		170.23				219-221			0.1 aq; 1.7 alc; 1.7
	capto-6-propyl-									acet; v s alk; i bz
	pyrimidine									
h130	2-Hydroxy-3-meth-	CH ₃ OC ₆ H ₃ (OH)CHO	152.15	8, 240			40-42	265-266		v s alc, eth; sl s aq
	oxybenzaldehyde									•
h131	4-Hydroxy-3-meth-	CH ₃ OC ₆ H ₃ (OH)CHO	152.15	8, 247	1.056		80-81	285		1 aq; s alc, chl, pyr
	oxybenzaldehyde									
h132	4-Hydroxy-3-meth-	CH ₃ OC ₆ H ₃ (OH)COOH	168.15	10, 392			210			0.12 aq; v s alc
	oxybenzoic acid									_

Hydroxyethanal, h86 3-(α-Hydroxyethyl)aniline, a261 *N*-(2-Hydroxyethyl)-3-aza-1,5-pentanediol, t264 N-(2-Hydroxyethyl)ethyleneimine, a321 N-(2-Hydroxyethyl)piperidine, p185 2-(2-Hydroxyethyl)piperidine, p186 *O*-Hydroxyethylresorcinol, h159 2-Hydroxyisobutyronitrile, h145 2-Hydroxy-3-methyl-2-cyclopenten-1-one, m214

h129

h128

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h133	4-Hydroxy-3-meth-	CH ₃ OC ₆ H ₃ (OH)CN	149.15	10, 398			85–87			
h134	oxybenzonitrile 2-Hydroxy-4-methoxybenzophenone	CH ₃ OC ₆ H ₃ (OH)COC ₆ H ₅	228.25	8, 312			66	155 ^{5mm}		v s alc, chl, eth
h135	4-Hydroxy-3-meth- oxybenzyl alcohol	CH ₃ OC ₆ H ₃ (OH)CH ₂ OH	154.17	6, 1113			113–115			
h136	4-Hydroxy-3-meth- oxycinnamic acid	CH ₃ OC ₆ H ₃ (OH)CH=CH- COOH	194.19	10, 436			174			s hot aq, alc, eth, EtAc; sl s bz, PE
h137	2-Hydroxy-3-methyl- benzoic acid	CH ₃ C ₆ H ₃ (OH)COOH	152.15	10, 220			165–166			s alc, chl, eth, alk
h138	2-Hydroxy-4-methyl- benzoic acid	CH ₃ C ₆ H ₃ (OH)COOH	152.15	10, 233			177			s alc, chl, eth, alk
h139	4-Hydroxy-3-methyl- 2-butanone	HOCH ₂ CH(CH ₃)COCH ₃	102.13	11,422	0.993	1.4340 ²⁰		92 ^{15mm}	78	
h140	7-Hydroxy-4-methyl-		176.17	18, 31			194–195			s alc, HOAc; sl s eth
h141	2-Hydroxymethyl-2- methyl-1,3- propanediol	HOCH ₂ C(CH ₃)(CH ₂ OH) ₂	120.09	1,520			199–203			
h142	4-Hydroxy-4-methyl- 2-pentanone	(CH ₃) ₂ C(OH)CH ₂ COCH ₃	116.16		0.9385^{20}	1.4235 ²⁰	-42.8	169	12	misc aq
h143	N-(Hydroxymethyl)- phthalimide		177.16	21, 475			142–145			sl s aq, alc, bz
h144	4-Hydroxy- <i>N</i> -methyl-		115.18	21 ¹ , 188		1.4775 ²⁰	29–31	200	>112	
h145	2-Hydroxy-2-methyl- propanenitrile	(CH ₃) ₂ C(OH)CN	85.10	3, 316	0.9267_4^{25}	1.399220	-19	95	63	s aq, alc, chl, eth

h146	3-Hydroxy-2-methyl- 4-pyrone		126.11			161–162		1.2 aq; v s hot aq; s alc, alk; sl s bz, eth
h147	2-Hydroxy-1-naph- thaldehyde	C ₁₀ H ₆ (OH)CHO	172.18	8, 143		82–85	192 ^{27mm}	, , ,
h148	1-Hydroxy-2-naph- thalenecarboxylic acid	C ₁₀ H ₆ (OH)COOH	188.18	10, 331		191–192		v s alc, bz, eth, alk
h149	3-Hydroxy-2-naph- thalenecarboxylic acid	C ₁₀ H ₆ (OH)COOH	188.18	10, 333		222–223		v s alc, eth; s bz, chl
h150	2-Hydroxy-3,6- naphthalenedi- sulfonic acid, disodium salt	C ₁₀ H ₅ (OH)(SO ₃ ⁻ Na ⁺) ₂	348.25	11, 288				v s aq, alc; i eth
h151	4-Hydroxy-2,7- naphthalenedi- sulfonic acid, disodium salt	C ₁₀ H ₅ (OH)(SO ₃ ⁻ Na ⁺) ₂	348.25	11, 227		>300		
h152	2-Hydroxy-1,4- naphthoquinone		174.16	8,300		d 185		s HOAc

3-Hydroxymethylpiperidine, p187

1-Hydroxy-2-napthoic acid, h148

3-Hydroxy-2-naphthoic acid, h149

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h153	4-Hydroxy-3-nitro- benzenearsonic acid	HOC ₆ H ₃ (NO ₂)- AsO(OH) ₂	263.04	16¹, 456			>300			v s alc, acet, HOAc, alk; sl s aq; i eth
h154	3-Hydroxy-4-nitro- benzoic acid	HOC ₆ H ₃ (NO ₂)COOH	183.12	10, 146			229–231			
h155	2-Hydroxy-5-nitro- benzyl bromide	HOC ₆ H ₃ (NO ₂)CH ₂ Br	232.04	6, 367			147–149			
h156	5-Hydroxy-1-pentanal	HO(CH ₂) ₄ CHO	102.13		1.055	1.4530^{20}		115 ^{15mm}	>112	s aq
h157	5-Hydroxy-2- pentanone	CH ₃ COCH ₂ CH ₂ CH ₂ OH	102.13	1,831	1.007_4^{20}	1.437220		144 ^{100mm}	93	misc aq; s alc, eth
h158	4-Hydroxy-3-penten- 2-one acetate	CH ₃ COOC(CH ₃)=CH- COCH ₃	142.15			1.4525 ²⁰		195	75	
h159	2-(<i>m</i> -Hydroxy- phenoxy)ethanol	HOC ₆ H ₄ OCH ₂ CH ₂ OH	154.17				83–86			
h160	4-Hydroxyphenyl- acetic acid	HOC ₆ H ₄ CH ₂ COOH	152.15	10, 190			149–151	subl		v s alc, eth; sl s aq
h161	2-Hydroxy- <i>N</i> -phenyl- benzamide	HOC ₆ H ₄ CONHC ₆ H ₅	213.14	12, 500			136			v s alc, bz, chl, eth
h162	4-(<i>p</i> -Hydroxphenyl)- 2-butanone	HOC ₆ H ₄ CH ₂ CH ₂ COCH ₃	164.20				82–83			
h163	D-(-)- <i>p</i> -Hydroxy- phenylglycine	HOC ₆ H ₄ CH(NH ₂)COOH	167.16	14 ¹ , 659			240 d			sl s aq, alc, bz, acet
h164	N-(p-Hydroxy- phenyl)glycine	HOC ₆ H ₄ NHCH ₂ COOH	167.16	13, 488			220– 248 d			s alk, acid; v sl s aq, alc, acet, bz, chl, eth
h165	1-(3-Hydroxyphenyl)- urea	HOC ₆ H ₄ NHCONH ₂	152.15	13, 417			182–184			

h166	N-Hydroxyphthal-		163.13	21,500			233 d			
h167	imide N-Hydroxypiper- idine		101.15	20, 80			37–40	111 ^{55mm}		
h168	2-Hydroxypropio- nitrile	CH₃CH(OH)CN	71.08	$3^2, 209$	0.9834 ²⁵	1.4027 ²⁵	-34	103 ^{50mm}	77	misc aq, alc; s eth
h169	3-Hydroxypropio- nitrile	HOCH ₂ CH ₂ CN	71.08	3, 298	1.0404_4^{25}	1.4256^{20}	-46	228	>112	misc aq, alc, acet; 2.3 eth; i bz, PE
h170	o-Hydroxypropio- phenone	HOC ₆ H ₄ COCH ₂ CH ₃	150.18	8, 102	1.094	1.5480^{20}		115 ^{15mm}	>112	v s alc, eth; sl s aq
h171	p-Hydroxypropio- phenone	HOC ₆ H ₄ COCH ₂ CH ₃	150.18	8, 102			148			v s alc, eth; sl s aq
h172	1-(2-Hydroxy-1-pro- poxy)-2-propanol	CH ₃ CH(OH)CH ₂ OCH ₂ - CH(OH)CH ₃	134.18		1.0252_{20}^{20}	1.4440^{20}		231.8	138	misc aq, alc
h173	2-Hydroxypyridine	HOC ₅ H ₄ N	95.10	21, 43			105–107	280–281		s aq, alc, bz; sl s eth
h174	3-Hydroxypyridine	HOC ₅ H ₄ N	95.10	21, 46			126-129	151 ^{3mm}		v s aq, alc; sl s eth
h175	4-Hydroxypyridine	HOC₅H₄N	95.10	21, 48				230 ^{12mm}		v s aq; i alc, bz, eth
h176	2-Hydroxypyridine- 5-carboxylic acid	HO(C₅H₃N)COOH	139.11	22, 215			>300			sl s aq, alc, eth

6-Hydroxynicotinic acid, h176 α -Hydroxy- α -phenylacetophenone, b46 3-(p-Hydroxyphenyl)alanine, t437

2-Hydroxy-2-phenylbenzeneacetic acid, b36 3-Hydroxy-1-propanesulfonic acid γ-sultone, p198 2-Hydroxypropanoic acids, L1, L2 1-Hydroxy-2-propanone, h89 3-Hydroxypropionitrile, c290

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h177	3-Hydroxypyridine- N-oxide	(HO)C ₅ H ₄ N=O	111.10				190–192			
h178	8-Hydroxyquinoline		145.16	21,91			76	267		v s alc, acet, bz,
h179	8-Hydroxyquinoline- 5-sulfonic acid		225.22	22, 407			213 d			v s aq; sl s alc, eth
h180	DL-Hydroxysuccinic acid	HOOCCH(OH)CH ₂ COOH	134.09	3, 435			131–133			56 aq; 45 EtOH: 18 acet; 0.8 eth;
h181	L-Hydroxysuccinic acid	HOOCCH(OH)CH₂COOH	134.09	3,419			100			23 diox; i bz 36 aq; 87 EtOH; 2.7 eth; 61 acet; 75 diox
h182	N-Hydroxy- succinimide		115.09	21, 380			93–95			v s aq
h183	6-Hydroxytetrahydro- pyran-2-carboxylic acid lactone		128.13		1.226	1.4593 ²⁰				
h184	3-Hydroxy-3,7,11- trimethyl-1,6,10- dodecatriene	H_2C =CHC(OH)(CH ₃)- CH ₂ CH ₂ CH=C(CH ₃)- CH ₂ CH,CH=C(CH ₃),	222.37		0.8760425	1.4769 ²⁵		114 ^{1mm}	96	s abs alc
h185	3-Hydroxy-2,2,4- trimethyl-3- pentenoic acid β-lactone		140.18		0.947	1.4380 ²⁰	-18	170	62	
h186	Hypoxanthine		136.11	26, 416			d 150			0.25 aq; s alk, acid
i1	1 <i>H</i> ,1 <i>H</i> ,11 <i>H</i> -Icosa-	HCF ₂ (CF ₂) ₉ CH ₂ OH	531.1	-,			95–97	181 ^{200mm}		
	fluoro-1-undecanol	2\ 2/9 2								
i2	Icosane	CH ₃ (CH ₂) ₁₈ CH ₃	282.56		0.7777^{37}	1.434640	36.4	343.8	>112	
i3	1-Icosene	$CH_3(CH_2)_{17}CH = CH_2$	280.54	1 ³ , 881			28.7	342.4		

i5 2-Imidazo	idinathi		68.08 102.16	23, 45			90–91 203–204	257	145	v s aq, alc, chl, eth 2 aq; s alc, pyr; i
one	idilicuii-		102.10	24,4			203-204			bz, acet, chl, eth
i6 Imidazolid	inetrione		114.06				230	subl 100		5 aq; s alc
i7 2-Imidazo	idone		86.09	24, 16			131			v s aq, hot alc
i8 2-(4-Imida	zolyl)		111.15	25, 315			83-84	209 ^{18mm}		v s aq, alc, hot chl
ethylam	ine									
i9 3,3'-Imino	bispropyl-	H ₂ NCH ₂ CH ₂ CH ₂ NHCH ₂ -	131.22		0.938	1.4810^{20}	-14	151 ^{50mm}	118	
amine		$CH_2CH_2NH_2$								
i10 Iminodiace	etic acid	HOOCCH ₂ NHCH ₂ COOH	133.10	4, 365			243 d			2 aq; v sl s bz, eth
ill Iminodiace	etonitrile	NCCH ₂ NHCH ₂ CN	95.11	4, 367			77			s aq, alc: sl s eth
i12 Iminodiber	nzyl		195.27				105-108			
i13 Indan			118.18		0.9639_4^{20}	1.5360^{20}	-51.4	176.5	50	s alc, chl, eth; i aq
i14 5-Indanol			134.18	6, 575			51-53	255		v s alc, eth; sl s aq
i15 1-Indanon	e		132.16	7, 360	1.1090_4^{45}	1.56145	40-42	243-245		s alc, eth; sl s aq

5-Hydroxyvaleraldehyde, h156 Imidodicarbonic diamide, b215 Indalone, b445

Indanamines, a199, a200

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i16	1,2,3-Indantrione		178.14				d 241			
	hydrate									
i17	Indene		116.16	5, 515	0.9968_4^{20}	1.5762^{20}	-1.8	181.6	78	misc alc, bz, chl,
:10	T., J., 1.		117.15	20, 304	1.0642	1.60960	52	253		eth
i18 i19	Indole Indole-3-acetic acid		117.15 175.19	.,	1.0643	1.609**	168–170	255		s hot aq, bz, eth
				22, 66						v s alc; s acet, eth
i20 i21	Indole-3-carbaldehyde		145.16	21, 313			195–198			-1
121	Indole-2,3-dione		147.13	21, 432			203.5 d			s hot aq, hot alc, alk
i22	Indoline		119.17	20, 257	1.063	1.5906 ²⁰		221	92	sl s aq
i23	Inositol		180.16	6^2 , 1157	1.752		225–227		-	14 ag; sl s ag; i eth
i24	Iodoacetamide	ICH,CONH,	184.96	2, 223			91–93			s hot aq
i25	Iodoacetic acid	ICH,COOH	185.95	2, 222			82-83			s aq, alc; v sl s eth
i26	3-Iodoaniline	IC ₆ H ₄ NH ₂	219.03	12,670	1.821	1.6820^{20}	25	146 ^{15mm}	>112	i aq; s alc, eth
i27	Iodobenzene	C ₆ H ₅ I	204.01	5, 215	1.838345	1.62118	-30	188.3	74	misc alc, chl, eth
i28	Iodobenzene diacetate	C ₆ H ₃ I(OOCCH ₃) ₂	322.10				163-165			
i29	2-Iodobenzoic acid	IC ₆ H₄COOH	248.02	9, 363	2.249_4^{25}		162			s alc, eth; sl s aq
i30	1-Iodobutane	CH ₃ CH ₂ CH ₂ CH ₂ I	184.02	1, 123	1.616_4^{20}	1.4999^{20}	-103.5	129-130	33	i aq; s alc, eth
i31	2-Iodobutane	CH ₃ CH ₂ CH(I)CH ₃	184.02		1.592_4^{20}	1.4991^{20}	-104.0	118-120	28	i aq; s alc, eth
i32	Iodocyclohexane	$C_6H_{11}I$	210.06	$5^2, 13$	1.626_{15}^{15}	1.5472^{20}		180		i aq; s eth
i33	1-Iododecane	CH ₃ (CH ₂) ₉ I	268.18	1, 168	1.257_4^{20}	1.4827^{20}		132 ^{15mm}		i aq; s alc, eth
i34	Iodoethane	CH ₃ CH ₂ I	155.97	1,96	1.9358^{20}	1.5137	-110.9	72.4	none	0.4 aq; misc alc,
										bz, chl, eth
i35	2-Iodoethanol	ICH ₂ CH ₂ OH	171.97	1, 339	2.2197_4^{20}	1.5694^{20}		75 ^{5mm}	65	s aq; v s alc, eth
i36	Iodoform	CHI ₃	393.73	1,73	4.008		120-123		none	1.4 alc; 10 chl; 13
										eth; v s bz, acet
i37	1-Iodoheptane	CH ₃ (CH ₂) ₆ I	226.10	1, 155	1.373_4^{20}	1.4900^{20}	-48.2	204	78	i aq; s alc, eth
i38	1-Iodohexadecane	CH ₃ (CH ₂) ₁₅ I	352.35	1, 172	1.121	1.4806^{20}		206-		
								207 ^{10mm}		

i39	1-Iodohexane	CH ₃ (CH ₂) ₅ I	212.08	1, 146	1.437420	1.4926^{20}		179.5	61	i aq
i40	Iodomethane	CH₃I	141.94	1, 69	2.2789_4^{20}	1.5308^{20}	-66.5	42.4	none	1.4 aq; misc alc, eth
i41	4-Iodomethoxyben- zene	IC ₆ H ₄ OCH ₃	234.04	6, 208			48–50	237 ^{726mm}		s hot alc, eth
i42	1-Iodo-3-methyl- butane	(CH ₃) ₂ CHCH ₂ CH ₂ I	198.06	1 ³ , 367	1.509420	1.4939^{20}		147.5		misc alc, eth; sl s
i43	1-Iodo-2-methyl- propane	(CH ₃) ₂ CHCH ₂ I	184.02	1, 128	1.603 ²⁰		-93.5	119		i aq; misc alc, eth
i44	2-Iodo-2-methyl- propane	(CH ₃) ₃ CI	184.02	1 ³ , 326	1.5710	1.4918^{20}	-38.2			d aq; misc alc, eth
i45	1-Iodo-3-nitrobenzene	IC ₆ H ₄ NO ₂	249.01	5, 253	1.9477_4^{50}		36-38	280		i aq; s alc, eth
i46	1-Iodooctane	CH ₃ (CH ₂) ₇ I	240.13	1, 160	1.330_4^{20}	1.4889^{20}	-45.9	221		s alc, eth
i47	1-Iodopentane	CH ₃ (CH ₂) ₄ I	198.06	1, 133	1.512_4^{20}	1.4954^{20}	-85.6	154.5	79	sl s aq; s alc, eth
i48	1-Iodopropane	CH ₃ CH ₂ CH ₂ I	169.99	1, 113	1.7489 ²⁰	1.5058^{20}	-101	102.5	none	0.1 aq; misc alc, eth

Indonaphthene, i17

ОН Ю O i16

i17

i18

4-Iodoanisole, i41

`CH₂COOH i19

> ОН OH∕он HÓ

ÓН i23 i22

5-Iodoanthranilic acid, a203

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i49	2-Iodopropane	(CH ₃) ₂ CHI	169.99	1, 114	1.7025420	1.499220	-90.0	89.5	none	0.14 aq; misc alc, bz, chl, eth
i50 i51	3-Iodo-1-propene 5-Iodosalicylic acid	ICH ₂ CH=CH ₂ IC ₆ H ₃ (OH)COOH	167.97 264.02	1 ³ , 114 10, 112	1.845422	1.5540 ²¹	-99 189-191	1–3		misc alc, chl, eth v s alc; i bz, chl
i52	2-Iodothiophene		210.04	17, 34	1.902	1.6520^{20}	-40	73 ^{15mm}	71	v s eth
i53	2-Iodotoluene	IC ₆ H ₄ CH ₃	218.04	5, 310	1.713	1.6079^{20}		211	90	i aq; s alc, eth
i54	3-Iodotoluene	IC ₆ H ₄ CH ₃	218.04	5, 311	1.698	1.6040^{20}		80 ^{10mm}	82	i aq; misc alc, eth
i55	Iodotrimethylsilane	(CH ₃) ₃ SiI	200.10		1.406_4^{20}	1.4710^{20}		106	<1	
i56	α-Ionone		192.30	7, 168	0.932^{20}	1.4980^{20}		124 ^{11mm}	104	s alc, bz, chl, eth
i57	β-Ionone		192.30	7, 167	0.94617	1.521^{17}		140 ^{18mm}	>112	s alc, bz, chl, eth
i58	Isatoic anhydride		163.13	27, 264			233 d			sl s aq, hot alc, acet
i59	D-(-)-Isoascrobic acid		176.12				169 d			s aq, alc, acet, pyr
i60	DL-Isoborneol		154.25	$6^2, 80$			212	subl		v s alc, chl, eth
i61	2-Isobutoxy-1-isobut- oxycarbonyl-1,2-di- hydroquinoline		303.40	·	1.022	1.5230 ²⁰		140 ^{0.2mm}	>112	
i62	Isobutyl acetate	(CH ₃) ₂ CHCH ₂ OOCCH ₃	116.16	2, 131	0.8745^{20}	1.3902^{20}	-98.9	118.0	25	0.7 aq; v s alc
i63	Isobutylamine	(CH ₃) ₂ CHCH ₂ NH ₂	73.14	4, 163	0.724_4^{20}	1.3972^{20}	-84.6	67.7	-26	misc aq, alc, acet, eth
i64	Isobutylbenzene	$C_6H_5CH_2CH(CH_3)_2$	134.22	5,414	0.8673_4^{20}	1.4855^{20}	-51.5	172.8	55	misc alc, eth
i65	Isobutyl	ClCOOCH ₂ CH(CH ₃) ₂	136.58	3, 12	1.053	1.4070^{20}		128.8	26	misc bz, chl, eth
	chloroformate	·								
i66	Isobutyl formate	HCOOCH ₂ CH(CH ₃) ₂	102.13	2, 21	0.8854_4^{20}	1.3855^{20}	-94.5	98.4	10	1 aq; misc alc, eth
i67	Isobutyl isobutyrate	(CH ₃) ₂ CHCH ₂ OOCCH- (CH ₃) ₂	144.22	2, 291	0.8542^{20}	1.3999^{20}	-80.7	147.5		0.5 aq; misc alc
i68	Isobutyl lactate	CH ₃ CH(OH)COOCH ₂ CH- (CH ₃) ₂	146.19	3 ² , 188	0.971_{20}^{20}	1.4181 ²⁵		96 ^{40mm}		

i69	Isobutyl methacrylate	$H_2C = C(CH_3)COOCH_2$	142.19		0.882_{15}^{25}	1.4170^{25}		155	45	misc alc, eth
		CH(CH ₃) ₂								
i70	Isobutyl nitrate	(CH ₃) ₂ CHCH ₂ ONO ₂	119.12		1.015_4^{20}	1.4028^{20}		123-125		i aq; misc alc, eth
i71	Isobutyl nitrite	(CH ₃) ₂ CHCH ₂ ONO	103.12	1,377	0.870_4^{22}	1.3715^{22}		67	4	misc alc; sl s aq(d)
i72	Isobutyl vinyl ether	$(CH_3)_2CHCH_2OCH = CH_2$	100.16		0.7702_{20}^{20}	1.3961^{20}	-132.3	83.4		0.2 aq
i73	Isobutyraldehyde	(CH ₃) ₂ CHCHO	72.11	1,671	0.7988_4^{20}	1.3723^{20}	-65.9	63-64	-40	11 aq; misc alc,
										bz, acet, chl, eth
i74	Isobutyramide	(CH ₃) ₂ CHCONH ₂	87.12	2, 293	1.013	127-129	216-220			
i75	Isobutyric acid	(CH ₃) ₂ CHCOOH	88.11	2, 288	0.950_4^{20}	1.3925^{20}	-46	154	55	17 aq; misc alc,
										chl, eth

Isatin, i21
Isethionic acid, h114
Isoamyl acetate, i80
Isoamyl alcohol, m155
sec-Isoamyl alcohol, m156
Isoamyl bromide, b305
Isoamyl iodide, i42
Isoamyl nitrite, i81

i52

CH₃ CH₃ O CH₃

i56

Isobutane, m375
Isobutene, m383 α -Isobutoxy- α -phenylacetophenone, b48
Isobutylacetylene, m352
Isobutyl alcohol, m381
Isobutyl bromide, b310
Isobutyl chloride, c161
Isobutyl chlorocarbonate, i65

i61

Isobutyl 1,2-dihydro-2-isobutoxy-1quinolinecarboxylate, i61 Isobutyl ether, d407 Isobutyl heptyl ketone, t349 Isobutyl mercaptan, m379 Isobutyraldehyde, m374 Isobutyramide, m388 Isobutyric acid, m390

1.277

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i76 i77	Isobutyronitrile Isobutyrophenone	(CH ₃) ₂ CHCN C ₆ H ₅ COCH(CH ₃) ₂	69.11 148.21	2, 294 7, 316	0.7704^{20} 0.988^{20}	1.3734 ²⁰ 1.5172	-71.5	103.8 217	3 84	v s alc, eth; sl s aq
i78	Isobutyryl chloride	(CH ₃) ₂ CHCOCl	106.55	2, 293	1.017	1.4073 ²⁰	-90	91–93	1	d aq, d alc; s eth
i79	L-Isoleucine	CH ₃ CH ₂ CH(CH ₃)CH- (NH ₂)COOH	131.18	4, 454			d 284	subl 168		4 aq; sl s hot alc
i80	Isopentyl acetate	CH ₃ COOCH ₂ CH ₂ - CH(CH ₃) ₂	130.19	2, 132	0.876_4^{15}	1.4007 ²⁰	-78.5	142.0	25	0.25 aq; misc alc, eth
i81	Isopentyl nitrite	(CH ₃) ₂ CHCH ₂ CH ₂ ONO	117.15	1,402	0.872	1.3860^{20}		99	10	misc alc, eth; sl s
										aq
i82	Isophorone		138.21	7, 65	0.923	1.4759^{20}	-8.1	215.2	84	1.2 aq
i83	DL-Isopinocampheol		154.25	6, 67			35–36	217		
i84	Isopropenyl acetate	$CH_3COOC(CH_3) = CH_2$	100.12	$2^2, 278$	0.909	1.4005 ²⁰		94	18	
i85	2-Isopropoxyphenol	(CH ₃) ₂ CHOC ₆ H ₄ OH	152.19	6 ³ , 4209	1.030	1.5157 ²⁰		100- 102 ^{11mm}		
i86	1-Isopropoxy-2- propanol	CH ₃ CH(OH)CH ₂ OCH- (CH ₃) ₂	118.1		0.879_{25}^{25}	1.407 ²⁵		47.9	49	
i87	Isopropyl acetate	(CH ₃) ₂ CHOOCCH ₃	102.13	2, 130	0.870_4^{20}	1.377320	-73.4	88.2	16	3 aq; misc alc, eth
i88	Isopropylamine	(CH ₃) ₂ CHNH ₂	59.11	4, 152	0.686^{25}_{4}	1.3711 ²⁵	-101	32.4	-17	misc aq, alc, eth
i89	2-Isopropylamino- ethanol	(CH ₃) ₂ CHNHCH ₂ CH ₂ OH	103.17	4, 282	0.8970_4^{20}	1.4395 ²⁰		75 ^{11mm}		misc aq, alc, eth
i90	2-Isopropylaniline	(CH ₃) ₂ CHC ₆ H ₄ NH ₂	135.2		0.966			222		
i91	Isopropylbenzene	C ₆ H ₅ CH(CH ₃) ₂	120.20	5, 393	0.864_4^{20}	1.4915^{20}	-96.0	152.4	46	s alc, bz, eth
i92	4-Isopropylbenzyl alcohol	(CH ₃) ₂ CHC ₆ H ₄ CH ₂ OH	150.22	6 ³ , 1911	0.98215	1.5206 ²⁰	28	248.4	>112	misc alc, eth; i aq
i93	N-Isopropylbenzyl-	C ₆ H ₅ CH ₂ NHCH(CH ₃) ₂	149.24		0.892	1.5025 ²⁰		200	87	
i94	Isopropylcyclohexane	$C_6H_{11}CH(CH_3)_2$	126.24	5, 41	0.8023_4^{20}	1.439920	-90	155	35	v s alc, eth
i95	N-Isopropylcyclo- hexylamine	C ₆ H ₁₁ NHCH(CH ₃) ₂	141.26		0.859	1.4480 ²⁰		60 ^{12mm}	33	

i96	4,4'-Isopropylidene- bis[2-(2,6-di- bromophenoxy)- ethanoll	(CH ₃) ₂ C[C ₆ H ₂ (Br) ₂ - OCH ₂ CH ₂ OH] ₂	632.01				107			
i97	4,4'-Isopropylidene- diphenol	(CH3)2C[C6H4OH]2	228.29	6, 1011			153–156	220 ^{4mm}		
i98 i99	Isopropyl isocyanate Isopropyl S-(-)- lactate	(CH ₃) ₂ CHCNO (CH ₃) ₂ CHOOC- CH(OH)CH ₃	85.11 132.16	4, 155 3, 282	$0.866 \\ 0.998_{20}^{20}$	1.3825 ²⁰ 1.4082 ²⁵		74–75 166–168	-2	s aq, alc, eth

Isocapronitrile, m339
Isocinchomeronic acid, p260
Isocrotonic acid, b401
Isodurene, t98
Isoeugenol, m98
Isohexane, m336
Isoleucinol, a216
Isoniazid, p258
Isonicotinaldehyde, p253
Isonicotine acid, p257
Isonicotinic acid hydrazide, p258
Isonicotinonitrile, c297
Isocapronitrile, c297

Isopentane, m149
Isopentyl alcohol, m155
Isopentyl isovalerate, m170
Isophorone, t340
Isophthalic acid, b16
Isophthalic acid, b16
Isophthalonitrile, d237
Isophthaloyl dichloride, b14
Isoprene, m147
Isopropanolamine, a269
Isopropenyl acetate, p208
Isopropenylacetylene, m166
4-Isopropenyl-1-cyclohexene-1-carbaldehyde, p58

Isopropenyl methyl ether, m96 Isopropylacetylene, m171 Isopropylacrylic acid, m349 Isopropyl alcohol, p203 Isopropyl chloride, c211 Isopropyl cyanide, i76 Isopropyl ether, d417 Isopropylethylene, m160 Isopropylidone acetone, m350 Isopropyl iodide, i49

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i100	2-Isopropyl-1-methyl- benzene	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.21	5, 419	0.8766_4^{20}	1.5006 ²⁰	-71.5	178.2		misc alc, eth
i101	3-Isopropyl-1-methyl- benzene	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.21	5, 419	0.8610_4^{20}	1.4930 ²⁰	-63.75	175.1		misc alc, eth
i102	4-Isopropyl-1-methyl- benzene	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.21	5, 420	0.8573_4^{20}	1.4909 ²⁰	-67.9	177.1	47	misc alc, eth
i102a	2-Isopropyl-5-methyl- phenol	CH ₃ C ₆ H ₃ (OH)- CH(CH ₃) ₂	150.22	6, 532	0.925_4^{80}		49–51	232		i aq; v s alc, chl, eth
i103	N ¹ -Isopropyl-2- methyl-1,2- propanedi- amine	(CH ₃) ₂ C(NH ₂)CH ₂ NH- CH(CH ₃) ₂	130.24		0.822	1.4269 ²⁰		147–149	90	
i104	Isopropyl methyl sulfide	(CH ₃) ₂ CHSCH ₃	90.18	1, 367			-101.5	84.7		
i105	Isopropyl nitrate	(CH ₃) ₂ CHONO ₂	105.09	1^3 , 1465	1.036_{19}^{19}	1.391216		102.1		
i106	2-Isopropylphenol	(CH ₃) ₂ CHC ₆ H ₄ OH	136.19	6, 504	1.012^{20}	1.5259^{20}	15–16	212–213	107	misc alc, eth
i107	4-Isopropylphenol	(CH ₃) ₂ CHC ₆ H ₄ OH	136.19	6, 505	0.990^{20}		59–61	212		316 alc; 350 eth
i108	Isopropyl vinyl ether	(CH ₃) ₂ CHOCH=CH ₂	86.13		0.753_4^{20}	1.3849 ²⁰	-140	5–6		
i109	Isopulegol		154.25	6, 65	0.911	1.4725^{20}		91 ^{12mm}	78	v sl s aq
i110	Isoquinoline		129.16	20, 380	1.0910_4^{30}	1.6208^{30}	26.5	243.2	107	sl s aq; s acid
k1	Ketene	$H_2C=C=O$	42.04	1,724			-151	-41		s acet, eth; d aq
L1	DL-Lactic acid	CH₃CH(OH)COOH	90.08	3, 268	1.249_4^{15}		16.8	122 ^{14mm}		s aq, alc; i chl
L2	L-(+)-Lactic acid	CH₃CH(OH)COOH	90.08	3, 261	1.2060_4^{25}	1.4392^{20}	53	119 ^{12mm}	>112	v s aq, alc, eth
L3	α-Lactose		342.30	31, 408	1.525^{20}		219 d			17 aq; i alc, eth
L4	DL-Leucine	(CH ₃) ₂ CHCH ₂ - CH(NH ₂)COOH	131.18	4, 447			d 332	subl 293		1 aq; 0.13 alc; i eth
L5	L-Leucine	(CH ₃) ₂ CHCH ₂ - CH(NH ₂)COOH	131.18	4, 437	1.29318		d 293	subl 145		2.4 aq; 0.07 alc; 1 HOAc; i eth

L6	(+)-Limonene		136.24	5, 133	0.8411_4^{20}	1.4715	-96.5	175–176	53	misc alc, eth
L7	(-)-Limonene		136.24	5, 136	0.844	1.4706^{20}	-96.5	175-176	48	misc alc, eth
L8	(+)-Limonene oxide		152.24	17, 44	0.929	1.4661^{20}		114 ^{50mm}	65	
L9	Linalool		154.25	1,462	0.865^{15}	1.4615^{20}		199	76	misc alc, eth
L10	Linalyl acetate		196.29	2, 141	0.895^{20}	1.451		220 d	84	misc alc, eth
L11	N-Lithiohexamethyl-	(CH ₃) ₃ SiN(Li)Si(CH ₃) ₃	167.3				70-72	115		
	disilazane									

Isopropyl mercaptan, p200
1-Isopropyl-4-methyl-1,3-cyclohexadiene, t5
1-Isopropyl-4-methyl-1,4-cyclohexadiene, t6
Isopropyl methyl ketone, m157
Isopropyltolueness, i100, i101, i102
Isopseudocumenol, t358
Isovaleraldehyde, m174
Isovaleric acid, m177
Isovaleronitrile, m178
Isovaleryl chloride, m179

Keto compounds, see Oxo
2-Ketobutyric acid, o56
5-Keto-1,7,7-trimethylnorcamphane, c3
4-Ketovaleric acid, o58
Koshland's reagent I, h155
Lactonitrile, h168
Lauraldehyde, d731
Lauric acid, d726
Lauronitrile, d724
Lauroyl chloride, d728
Lauryl alcohol, d727

Laurylamine, d732 Lauryl bromide, b275 Lauryl mercaptan, d725 Lauryl sulfate, d735 Lepidine, m408 Leucinol, a217 Levulinic acid, o58 Linoleic acid, o1 Linolenic acid, o7

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
L12	L-(+)-Lysine	H ₂ N(CH ₂) ₄ - CH(NH ₂)COOH	146.19	4, 435			d 224			v s aq; sl s alc; i eth
m1 m2	Maleic acid Maleic anhydride	HOOCCH=CHCOOH	116.07 98.06	2,748 17,432	1.590 1.48		138–139 52.8	202.0	103	79 aq; 70 alc; 8 eth s aq (to acid), alc (to ester); 227 acet; 53 chl; 50 bz; 112 EtAc
m3	Malonic acid	HOOCCH ₂ COOH	104.06	2, 566	1.63		135 d			154 aq; 42 alc; 8 eth
m4	Malonodiamide	H ₂ NCOCH ₂ CONH ₂	102.09	2, 582			168–170			9 aq; i alc, eth
m5	Malononitrile	NCCH ₂ CN	66.06	2, 589	1.049		32–34	220	112	13 aq; 40 alc; 20 eth
m6	Malonyl dichloride	ClCOCH ₂ COCl	140.95	21, 252	1.448649	1.462020		53 ^{19mm}	47	d hot aq; s eth
m7	D-(+)-Maltose hydrate		342.30	31,386	1.54017		102–103	d 130		v s aq; sl s alc; i eth
m8	D-Mandelic acid	C ₆ H ₅ CH(OH)COOH	152.15	10, 197	1.300_4^{20}		119	d		16 aq; 100 alc; s eth
m9	Mandelonitrile	C ₆ H ₅ CH(OH)CN	133.15	10, 193	1.117	1.5315 ²⁰	-10	d 170		v s alc, chl, eth; i
m10 m11	Mannitol D-(+)-Mannose		182.17 180.16	1,534 31,284	$ \begin{array}{c c} 1.52^{20} \\ 1.54^{20} \end{array} $		166–168 128–130	290 ^{3.5mm}		aq 18 aq; 1.2 alc; i eth 250 aq; 28 pyr; 0.8 alc
m12 m13	L-Menthol L-Menthone		156.27 154.25	6, 28 7, 38	$\begin{bmatrix} 0.890^{15}_{15} \\ 0.895^{20}_{4} \end{bmatrix}$	$ \begin{array}{c} 1.458^{25} \\ 1.4510^{20} \end{array} $	43–45 –6	212 207	93 69	v s alc, chl, eth, PE misc alc, eth; sl s
m14	Mercaptoacetic acid	HSCH₂COOH	92.12	3, 245	1.325	1.5030 ²⁰	-16.5	96 ^{5mm}	>112	misc aq, alc, bz,
m15	2-Mercaptobenzimid- azole		150.20	24, 119			303–304			sl s aq; s alc

m16	o-Mercaptobenzoic	HSC ₆ H ₄ COOH	154.19	10, 125			164–165			v s alc, HOAc
m17	2-Mercaptobenzo- thiazole		167.25	27, 185	1.42 ²⁰		180–181	d		2 alc; 1 eth; 10 acet; 1 bz; s alk; i aq
m18	2-Mercaptoethanol	HSCH ₂ CH ₂ OH	78.13	1,470	1.1143420	1.5006 ²⁰		156.9	73	misc aq, alc, bz,
m19	2-Mercaptoethyltri- ethoxysilane	HSCH ₂ CH ₂ Si(OC ₂ H ₅) ₃	224.38		0.988_4^{20}	1.43220		210	104	

Luminol, a153 2,6-Lupetidine, d591 β-Lutidine, e212 Lutidines, d604, d605, d606, d607 Maleic hydrazide, d400 Malic acids, h180, h181 Malonaldehyde bis(dimethyl acetal), t91 Malonamide nitrile, c286 Malonic acid diamide, m4 Malonylurea, b1 Melamine, t198 Mellitic acid, b19 MEM chloride, m67 Menadione, m310 1,8-Mentanediamine, d41 p-Mentha-1,8-diene, d649 p-Mentha-6,8-dien-2-one, c20 Mercaptobenzene, t159

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m20	3-Mercapto-1,2- propanediol	HSCH ₂ CH(OH)CH ₂ OH	108.16	1,519	1.29514	1.5243 ²⁰		118 ^{5mm}	>112	misc alc; v s acet
m21	2-Mercaptopropionic acid	CH₃CH(SH)COOH	106.14	3, 289	1.220_4^{15}	1.4809 ²⁰	10	117 ^{16mm}	87	misc aq, alc, eth, acet
m22	(3-Mercaptopropyl)- trimethoxysilane	HS(CH ₂) ₃ Si(OCH ₃) ₃	196.34		1.039_4^{20}	1.4416 ²⁰		93 ^{40mm}	48	
m23	Mercaptosuccinic acid	HOOCCH ₂ CH(SH)COOH	150.15	3, 439			152–154			50 aq; 50 alc; s eth
m24	Methacrylaldehyde	$H_2C = C(CH_3)CHO$	70.09	1,731	0.8304_4^{20}	1.4160^{20}	-81	69	-15	6 aq; misc alc, eth
m25	Methacrylamide	$H_2C = C(CH_3)CONH_2$	85.11	$2^2,399$			109-111			s alc; sl s eth
m26	Methacrylic acid	$H_2C = C(CH_3)COOH$	86.09	2, 421	1.0153_4^{20}	1.4314^{20}	16	163	76	9 aq; misc alc, eth
m27	Methacrylonitrile	$H_2C = C(CH_3)CN$	67.91	2,423	0.8001_4^{20}	1.4007 ²⁰	-35.8	90.3	12	2.6 aq; misc acet, bz
m28	Methacryloyl chloride	H ₂ C=C(CH ₃)COCl	104.54	$2^2,394$	1.070	1.4447 ²⁰		95–96	2	
m29	Methane	CH ₄	16.04	1,56	0.4240 ^{bp} 0.7168 g/L		-182.5	-161.5		3.3 mL aq; 47 mL alc
m30	Methanesulfonic acid	CH ₃ SO ₃ H	96.10	4, 4	1.481218	1.430320	20	167 ^{10mm}	>112	1.5 bz; misc aq
m31	Methanesulfonic anhydride	(CH ₃ SO ₂) ₂ O	174.19	,	4		71	138 ^{10mm}		v s aq(d)
m32	Methanesulfonyl chloride	CH₃SO₂Cl	114.55	4, 5	1.480548	1.4518 ²⁰	-32	161	110	s alc, eth
m33	Methanethiol	CH ₃ SH	48.11	1,288	0.8665_4^{20}		-123.0	6.0		2.3 aq; v s alc, eth
m34	Methanol	CH ₃ OH	32.04	1, 273	0.7913_4^{20}	1.3284 ²⁰	-97.7	64.7	11	misc aq, alc, bz, chl, eth

2.5	laci ii	CIT OD	1 22.05	13 1106	0.010720	1 227020	110	1 65 5	Laa	l e a a
m35	Methanol-d	CH ₃ OD	33.05	1 ³ , 1186	0.8127_4^{20}	1.3270^{20}	-110	65.5	11	misc aq, alc, eth
m36	Methanol- d_4	CD ₃ OD	36.07	1 ³ , 1187	0.888	1.3256^{20}		65.4	11	misc aq, alc, eth
m37	DL-Methionine	CH ₃ SCH ₂ CH ₂ - CH(NH ₂)COOH	149.21	$4^2,938$	1.340		281 d			3 aq; i eth; v sl s
m38	Methoxyacetic acid	CH ₃ OCH ₂ COOH	90.08	3, 232	1.174	1.4158^{20}		202-204	>112	misc aq, alc, eth
m39	o-Methoxyaceto-	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8, 85	1.090^{20}_{4}	1.5393^{20}		131 ^{18mm}	108	mise aq, aic, cui
11139	phenone	CH ₃ OC ₆ H ₄ COCH ₃	150.16	0,03	1.0904	1.5595		131	100	
m40	m-Methoxyaceto-	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8, 86	1.094	1.5410^{20}		239–241	110	s aq
	phenone									
m41	<i>p</i> -Methoxyaceto- phenone	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8,87	1.08241	1.5335^{20}	36–38	154 ^{26mm}		v s alc, eth
m42	2-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 358	1.09815	1.5730^{20}	5	225	98	i ag; misc alc, eth
m43	3-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 404	1.096	1.5794^{20}	1	251	>112	s alc, acid; sl s aq
m44	4-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 435	1.087	1.5771	60	243	- 112	v s alc; sl s aq
m45	2-Methoxybenz-	CH ₃ OC ₆ H ₄ CHO	136.15	8, 43	1.127	1.560^{20}	35–36	236	117	sl s alc, bz; i eth
11143	aldehyde	C113OC6114C11O	150.15	0,43	1.127	1.500	33–30	230	117	sis aic, oz, i cui
m46	4-Methoxybenz-	CH₃OC₀H₄CHO	136.15	8, 67	1.119	1.5713^{20}	-1	248	108	misc alc
	aldehyde									
m47	4-Methoxybenzamide	CH ₃ OC ₆ H ₄ CONH ₂	151.17	10 ² , 100			164-167	295		s aq; v s alc; sl s
		3 0 7 2		,						eth
m48	Methoxybenzene	C ₆ H ₅ OCH ₃	108.14	6, 138	0.9942^{20}	1.5170^{20}	-37.5	153.8	51	1 aq; misc alc, eth
m49	4-Methoxybenzene-	CH ₃ OC ₆ H ₄ SO ₂ Cl	206.65	11, 243			40-43			d aq; s alc, eth
	sulfonyl chloride	3 0 . 2								
m50	2-Methoxybenzoic	CH₃OC ₆ H₄COOH	152.15	10, 64	1.180		100	200		0.5 aq; v s alc, eth
	acid									1,
	[l .	I	1		l	I	I	

MES, m451 Mesidine, t330 Mesitol, t362 Mesitylene, t335 Mesityl oxide, m350 Mesoxylurea, a79 Mesyl chloride, m32 Metanilic acid, a119 Methacholine chloride, a49 Methacrolein, m24 Methallyl alcohol, m385 Methallyl chloride, c164

Methanal, f27 Methanoic acid, f32 Methenamine, h52 Methone, d508 4-Methoxy-2-butanone dim

4-Methoxy-2-butanone dimethyl acetal, t321

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m51	3-Methoxybenzoic acid	CH ₃ OC ₆ H ₄ COOH	152.15	10, 137			104	172 ^{10mm}		s hot aq, alc, eth
m52	4-Methoxybenzoic acid	CH ₃ OC ₆ H ₄ COOH	152.15	10, 154	1.3854		185	275–280		0.04 aq; v s alc, chl
m53	4-Methoxybenzoyl chloride	CH ₃ OC ₆ H ₄ COCl	170.60	10, 163		1.5810 ²⁰	22	145 ^{14mm}	87	i aq(d); s alc(d); s bz, acet
m54	4-Methoxybenzyl alcohol	CH ₃ OC ₆ H ₄ CH ₂ OH	138.17	6, 897	1.109_4^{25}	1.5442 ²⁰	23–25	259	>112	i aq; s alc, eth
m55	4-Methoxybenzyl-	CH ₃ OC ₆ H ₄ CH ₂ NH ₂	137.18	13,606	1.05015	1.546220		236–237	>112	v s aq, alc, eth
m56	2-Methoxybiphenyl	CH ₃ OC ₆ H ₄ C ₆ H ₅	184.24	6,672	1.023	1.6105^{20}		274	>112	
m57	3-Methoxy-1-butanol	CH ₃ OCH(CH ₃)CH ₂ - CH ₂ OH	104.15		0.9229_{20}^{20}	1.4145 ²⁰	-85	161.1	46	misc aq
m58	4-Methoxy-3-buten- 2-one	CH ₃ OCH=CHCOCH ₃	100.12		0.982	1.4660 ²⁰		200	63	
m59	1-Methoxy-1-buten- 3-yne	CH₃OCH=CHC≡CH	82.10		0.906_4^{20}	1.4818 ²⁰		122–125	8	v s org solv
m60	4-Methoxycinnamic acid	CH ₃ OC ₆ H ₄ CH=CHCOOH	178.19	10, 298			172–187			s CCl ₄
m61	1-Methoxy-1,3-cyclo- hexadiene		110.16	$6^3, 367$	0.929	1.4885 ²⁰		40 ^{15mm}	26	
m62	1-Methoxy-1,4-cyclo- hexadiene		110.16	$6^3, 367$	0.940	1.4819 ²⁰		148–150	36	
m63	7-Methoxy-3,7-di- methyloctanal	(CH ₃) ₂ C(OCH ₃)CH ₂ - CH ₂ CH(CH ₃)CH ₂ CHO	186.30		0.877	1.4374 ²⁰		60 ^{0.45mm}	98	
m64	2-Methoxy-1,3- dioxolane		104.11	19 ⁴ , 617	1.092	1.4091 ²⁰		129–130	31	
m65	2-Methoxyethanol	CH ₃ OCH ₂ CH ₂ OH	76.10	1,467	0.9646 ²⁰	1.4021 ²⁰	-85.1	124.6	46	misc aq

m66	2-(2-Methoxyethoxy)- ethanol	CH ₃ OCH ₂ CH ₂ OCH ₂ - CH ₂ OH	120.15		1.035_4^{20}	1.4264 ²⁰	-50	194.1	83	misc aq, alc, bz, eth, ketones
m67	2-Methoxyethoxy- methyl chloride	CH ₃ OCH ₂ CH ₂ OCH ₂ Cl	124.57		1.091	1.4270^{20}		50 ^{13mm}	>112	etti, ketones
m68	2-Methoxyethyl acetate	CH ₃ COOCH ₂ CH ₂ OCH ₃	118.13	2, 141	1.0049 ²⁰	1.402220	-65.1	144.5	43	misc aq
m69	2-Methoxyethylamine	CH3OCH3CH3NH3	75.11	$4^2,718$	0.864	1.4054^{20}		95	9	v s aq, alc
m70	1-Methoxy-2-indanol	3 - 2 - 2 - 2	164.20	6,970		1.5482^{20}		146 ^{11mm}	>112	1,
m71	2-Methoxy-5-methyl- aniline	CH ₃ OC ₆ H ₃ (CH ₃)NH ₂	137.18	13 ² , 388			52–54	235		s aq; v s alc, bz, eth
m72	3-Methoxy-4-methyl- aniline	CH ₃ OC ₆ H ₃ (CH ₃)NH ₂	137.18	13, 574			51–54	250–252		
m73	4-Methoxy-2-methyl- aniline	CH ₃ OC ₆ H ₃ (CH ₃)NH ₂	137.18	$13^2, 330$	1.065	1.5647 ²⁰	13–14	248–249	>112	s alc
m74	(4 <i>S</i> ,5 <i>S</i>)-(-)-4- Methoxymethyl-2-		205.26			1.5155 ²⁰		79 ^{0.05mm}		
	methyl-5-phenyl-2- oxazoline									
m75	4-Methoxy-4-methyl- 2-pentanone	(CH ₃) ₂ C(OCH ₃)CH ₂ - COCH ₃	130.18		0.906	1.4181 ²⁵			61	misc aq
m76	1-Methoxynaph-	$C_{10}H_7OCH_3$	158.20	6,606	1.090	1.6220^{20}		135 ^{12mm}	>112	
	thalene									

Methoxyethane, e171

2-Methoxyethoxychloromethane, m67

OCH₃ OCH₃ OCH₃ OCH₃ OCH₃ OCH₃ OCH₃
$$0$$
CH₃ OCH₃ 0 CH₃ OCH₃ 0 CH₃ OCH₃ 0 CH₃ OCH₃ 0 CH₃ 0 CH

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m77	2-Methoxynaph- thalene	C ₁₀ H ₇ OCH ₃	158.20	6, 640			72	272		s bz, eth, CS ₂
m78	2-methoxy-4-nitro- aniline	CH ₃ OC ₆ H ₃ (NO ₂)NH ₂	168.15	13, 390			138–140			
m79	2-Methoxy-5-nitro- aniline	CH ₃ OC ₆ H ₃ (NO ₂)NH ₂	168.15	13, 389	1.207156		117–119			s alc, hot bz, HOAc
m80	4-Methoxy-2-nitro-	CH ₃ OC ₆ H ₃ (NO ₂)NH ₂	168.15	13, 521			123–126			sl s aq; s alc, eth
m81	2-Methoxynitro- benzene	CH ₃ OC ₆ H ₄ NO ₂	153.14	6, 217	1.2527 ₄ ²⁰	1.5619^{20}	9.4	277	>112	0.17 aq; s alc, eth
m82	4-Methoxynitro- benzene	CH ₃ OC ₆ H ₄ NO ₂	153.14	6, 230	1.233		54	260		i aq; v s alc, eth
m83	4-Methoxy-3-nitro- benzoic acid	CH ₃ OC ₆ H ₃ (NO ₂)COOH	197.15	10, 181			186–189			
m84	2-Methoxy-5-nitro- pyridine	CH ₃ OC ₅ H ₃ N(NO ₂)	154.13	212, 33			108–109			
m85	4-Methoxy-2-nitro- toluene	CH ₃ OC ₆ H ₃ (NO ₂)CH ₃	167.16	6, 411	1.207	1.5525^{20}	17	267	>112	
m86	p-Methoxypheneth- ylamine	CH ₃ OC ₆ H ₄ CH ₂ CH ₂ NH ₂	151.21	13, 626		1.5379^{20}		138 ^{20mm}		
m87	2-Methoxyphenol	CH₃OC ₆ H₄OH	124.14	6, 768	1.112 (liquid)	1.5429	28	205	82	1.5 aq; misc alc,
m88	3-Methoxyphenol	CH ₃ OC ₆ H ₄ OH	124.14	6, 813	1.131	1.5510^{20}	<-17.5	115 ^{5mm}	>112	misc alc, eth; sl s
m89 m90	4-Methoxyphenol 3-(4-Methoxyphenoxy)-1,2-propanediol	CH ₃ OC ₆ H ₄ OH CH ₃ OC ₆ H ₄ OCH ₂ CH(OH)- CH ₂ OH	124.14 198.22	6, 843 6 ³ , 4411			55–57 76–80	243		v s bz; s alk

m91	4-Methoxyphenyl-	CH ₃ OC ₆ H ₄ CH ₂ COOH	166.18	10, 190			86–88	140 ^{3mm}		i aq; v s alc; s eth
m92	acetic acid o-Methoxyphenyl- acetone	CH ₃ OC ₆ H ₄ CH ₂ COCH ₃	164.20	8 ³ , 397	1.054	1.5250^{20}		130 ^{10mm}	>112	s alc, eth
m93	(o-Methoxyphenyl)- acetonitrile	CH ₃ OC ₆ H ₄ CH ₂ CN	147.18	10, 188			65–68	143 ^{15mm}		s hot bz
m94	2-Methoxy-p- phenylenediamine sulfate	$CH_3OC_6H_3(NH_2)_2 \cdot H_2SO_4$	236.26	13 ³ , 1349			283 d			
m95	1-Methoxy-2- propanol	CH ₃ OCH ₂ CH(OH)CH ₃	90.1		0.919_{20}^{20}	1.4021 ²⁰	-97	120.1	38	misc aq, acet, bz, eth
m96 m97	2-Methoxypropene trans-1-Methoxy-4-	$CH_3C(OCH_3)=CH_2$	72.11	1, 435	0.753	1.3820^{20}		34–36	-18	
11177	(1-propenyl)ben- zene	CH ₃ OC ₆ H ₄ CH=CHCH ₃	148.21	6, 566	0.9883420	1.5615 ²⁰	21.4	237	90	misc chl, eth; 50 alc; s bz, EtAc
m98	2-Methoxy-4- propenylphenol	CH ₃ OC ₆ H ₃ (OH)- CH=CHCH ₃	164.20	6, 955	1.087 ₄ ²⁰	1.5748 ²⁰	-10	266	>112	misc alc, eth; sl s
m99	2-Methoxy-4-(2- propenyl)phenol	CH ₃ OC ₆ H ₃ (OH)- CH ₂ CH=CH ₂	164.20	6, 961	1.0664 ₄ ²⁰	1.5408 ²⁰	-9.2	255	>112	misc alc, chl, eth; s HOAc, alk; i aq
m100	<i>p</i> -Methoxyprop-iophenone	CH ₃ OC ₆ H ₄ COCH ₂ CH ₃	164.20	8, 103	1.071	1.5465 ²⁰	27–29	273–275	>112	uq
m101 m102	2-Methoxypyridine 2-Methoxytetra- hydrofuran	CH ₃ OC ₅ H ₄ N	109.13 102.13	21, 44 17 ⁴ , 1019	1.038 0.972	$1.5029^{29} 1.4119^{20}$		142 105–107	32 7	misc aq

 α -Methoxy- α -phenylacetophenone, b49

6-Methoxytetralin, m103

Methoxy-1-tetralone, d358

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m103	6-Methoxy-1,2,3,4- tetrahydro- naphthalene		162.23	6 ² , 537		1.5402 ²⁰		90 ^{1mm}	>112	
m104	6-Methoxy-1- tetralone		176.22	$9^2,889$			77–79	171 ^{11mm}		
m105 m106 m107 m108	2-Methoxytoluene 3-Methoxytoluene 4-Methoxytrimethyl- silane	CH ₃ OC ₆ H ₄ CH ₃ CH ₃ OC ₆ H ₄ CH ₃ CH ₃ OC ₆ H ₄ CH ₃ CH ₃ OSi(CH ₃) ₃	122.17 122.17 122.17 104.2	6, 352 6, 376 6, 392	$\begin{array}{c} 0.9851_{15}^{15} \\ 0.9697_{25}^{25} \\ 0.969_{25}^{25} \\ 0.7560_{4}^{20} \end{array}$	$ \begin{array}{c} 1.5161^{20} \\ 1.5131^{20} \\ 1.5112^{20} \\ 1.3678^{20} \end{array} $		170–172 175–176 174 57–58	51 54 53	i aq; v s alc, eth s alc, bz, eth; i aq s alc, eth; i aq
m109	Methoxytripropyl- silane	CH ₃ OSi(C ₃ H ₇) ₃	188.4		0.822_4^{20}	1.428 ²⁰		83 ^{12mm}		
m110 m111	N-Methylacetamide Methyl acetate	CH ₃ CONHCH ₃ CH ₃ COOCH ₃	73.10 74.08	4, 58 2, 224	$0.9460^{35} \\ 0.9342_4^{20}$	1.4253 ³⁵ 1.3619 ²⁰	30.6 -98.1	206 56.3	-16	s aq 24 aq; misc alc, eth
m112 m113	Methyl acetoacetate p-Methylaceto- phenone	CH ₃ COCH ₂ COOCH ₃ CH ₃ C ₆ H ₄ COCH ₃	116.12 134.18	3, 632 7, 307	1.0747 ²⁰ 1.0051	1.4186 ²⁰ 1.5328 ²⁰	-80 22-24	171.7 226	70 92	50 aq; misc alc i aq; v s alc, eth
m114 m115	Methyl acrylate Methylamine	H ₂ C=CHCOOCH ₃ CH ₃ NH ₂	86.09 31.06	2, 399 4, 32	$0.9561_4^{20} \\ 0.699_4^{-11}$	1.411718	-76.5 -93.5	80.2 -6.3	6 0	6 aq; s alc, eth 959 mL aq; 10.5 bz; s alc; misc eth
m116	Methyl 2-amino- benzoate	H ₂ NC ₆ H ₄ COOCH ₃	151.17	14, 317	1.6849	1.5820 ²⁰	24	256	104	sl s aq; v s alc, eth
m117	2-(N-Methylamino)- benzoic acid	CH₃NHC₀H₄COOH	151.17	14, 323			170–172 d			0.2 aq; s alc, eth
m118	Methyl 3-amino- crotonate	CH ₃ C(NH ₂)=CHCOOCH ₃	115.13	3, 632			81–83			

m119	2-(Methylamino)- ethanol	CH ₃ NHCH ₂ CH ₂ OH	75.11	4, 276	0.937^{20}	1.4387^{20}		155–156	72	misc aq, alc, eth
m120	4-Methylamino- phenol sulfate	$(CH_3NHC_6H_4OH)_2$ · H_2SO_4	344.39	13, 442			260 d			4 aq; sl s alc; i eth
m121	2-(Methylamino)- pyridine	CH ₃ NHC ₅ H ₄ N	108.14	22 ¹ , 629	1.052_{29}^{29}	1.5785^{20}	15	201	87	s aq; v s alc, eth
m122 m123	N-Methylaniline N-Methylanilinium	C ₆ H ₅ NHCH ₃ C ₆ H ₅ NHCH ₃ ·HOOCCF ₃	107.16 221.18	12, 135	0.989_4^{20}	1.5704^{20}	-57 65-66	196	73	sl s aq; s alc, eth
111123	trifluoroacetate	C ₆ H ₅ IVHCH ₃ ·HOOCCF ₃	221.10				03-00			
m124	2-Methylanthra- quinone		222.24	7, 809			177	subl		v s bz; s alc, eth
m125	Methylarsonic acid	CH ₃ AsO(OH) ₂	139.96	4, 613			161			v s aq; s alc
m126	4-Methylbenz- aldehyde	CH ₃ C ₆ H ₄ CHO	120.15	7, 297	1.0194_4^{17}	1.5447 ²⁰		205	80	misc alc, eth; sl s
m127	Methyl benzene- sulfonate	C ₆ H ₅ SO ₂ OCH ₃	172.20	11 ² , 20	1.28894	1.5151 ²⁰	-4	154 ^{20mm}		v s alc, chl, eth
m128	2-Methylbenz- imidazole		132.17	23, 145			176–177			s alk, hot aq; sl s alc
m129	Methyl benzoate	C ₆ H ₅ COOCH ₃	136.15	9, 109	1.093345	1.520515	-12.1	199.5	82	0.2 aq; misc alc, eth

Methylal, d441
Methyl alcohol, m34
Methylaminoacetaldehyde dimethyl acetal, d442
α-(1-Methylaminoethyl)benzyl alcohols, e1, e2

2-Methyl-*p*-anisidine, m71 4-Methyl-*m*-anisidine, m72 5-Methyl-*o*-anisidine, m73 Methylanisoles, m105, m106, m107 Methyl anthranilate, m116 Methylanthranilic acids, a211, a212 N-Methylanthranilic acid, m117 Methylbenzene, t167 4-Methylbenzenesulfonic acid, t176

1.29

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m130	2-Methylbenzoic	CH ₃ C ₆ H ₄ COOH	136.15	9, 462	1.062		107–108	258–259		sl s aq; v s alc
m131	acid 3-Methylbenzoic acid	CH ₃ C ₆ H ₄ COOH	136.15	9, 475	1.054		111–113	263		0.09 aq; v s alc
m132	4-Methylbenzoic acid	CH₃C ₆ H₄COOH	136.15	9, 483			180–182	274–275		v s alc, eth
m133	2-Methylbenzo- phenone	CH ₃ C ₆ H ₄ COC ₆ H ₅	196.25	7, 439	1.083	1.5958 ²⁰	<-18	309–311	>112	v s alc, org solv
m134	4-Methylbenzo- phenone	CH ₃ C ₆ H ₄ COC ₆ H ₅	196.25	7, 440			59–60	326		v s bz, eth
m135	2-Methylbenzo- thiazole		149.22	27, 46	1.173	1.6170 ²⁰	12–14	238	102	s alc, HOAc; i aq
m136	5-Methyl-1 <i>H</i> -benzo- triazole		133.15	26, 58			80–82	210– 212 ^{12mm}		
m137	2-Methylben-		133.15	27, 46	1.121	1.549720	8.5–10	178	75	
m138	zoxazole α-Methylbenzyl	C ₆ H ₅ CH(CH ₃)OH	122.17	6, 475	1.019143	1.5211 ²⁰	21	204	85	v s alc; s bz, chl
m139	alcohol 3-Methylbenzyl alcohol	CH ₃ C ₆ H ₄ CH ₂ OH	122.17	6, 494	0.91617	1.5334 ²⁰	<-20	217		5 aq; s alc, eth
m140	4-Methylbenzyl alcohol	CH ₃ C ₆ H ₄ CH ₂ OH	122.17	6, 498			59–61	217		s alc, eth; sl s aq
m141	DL-α-Methylbenzyl- amine	C ₆ H ₅ CH(CH ₃)NH ₂	121.18	12, 1094	0.940	1.5254 ²⁰		185	79	
m142	4-Methylbenzylamine	CH ₃ C ₆ H ₄ CH ₂ NH ₂	121.18	12, 1141	0.952	1.5340 ²⁰	12–13	195	75	
m143	Methyl bromoacetate	BrCH ₂ COOCH ₃	152.98	2, 213	1.616	1.4586^{20}		52 ^{15mm}	62	s alc
m144	DL-Methyl-	CH ₃ CH ₂ CH(Br)COOCH ₃	181.04	2, 282	1.573			137-		
	2-bromobutyrate							138 ^{50mm}		

m145	Methyl 4-bromo-	BrCH ₂ CH=CHCOOCH ₃	179.02	I	1.522	1.4980^{20}		85 ^{13mm}	91	ı
111143	crotonate	BICH ₂ CH—CHCOOCH ₃	179.02		1.322	1.4900		0.5	91	
m146	Methyl 2-bromo- propionate	CH ₃ CH(Br)COOCH ₃	167.01	2, 253	1.497	1.5420^{20}		51 ^{19mm}	51	s alc
m147	2-Methyl-1,3- butadiene	$H_2C = C(CH_3)CH = CH_2$	68.12	1, 252	0.681420	1.4216^{20}	-145.9	34. 1	-53	misc alc, eth
m148	3-Methyl-1,2- butadiene	$CH_3C(CH_3) = C = CH_2$	68.12	1, 252	0.694_4^{20}	1.4179^{20}	-113.6	40.9	-12	
m149	2-Methylbutane	CH ₃ CH ₂ CH(CH ₃) ₂	72.15	1, 134	0.6197^{20}	1.3537^{20}	-159.9	27.9	-56	0.005 aq; misc alc
m150	2-Methyl-1- butanethiol	CH ₃ CH ₂ CH(CH ₃)CH ₂ SH	104.22	1 ² , 421	0.848	1.4465^{20}		119.0	19	s alc, eth; i aq
m151	2-Methyl-2-	CH ₃ CH ₂ C(CH ₃) ₂ SH	104.22	1 ¹ , 196	0.842	1.438520	-103.9	99.1	-1	s alc, eth; i aq
111131	butanethiol	C113C112C(C113)2S11	104.22	1,170	0.042	1.7303	103.7	77.1	1	s arc, cur, r aq
m152	3-Methyl-1- butanethiol	(CH ₃) ₂ CHCH ₂ CH ₂ SH	104.22	1,405	0.835_4^{20}	1.4432^{20}	-133.5	118.4	18	misc alc, chl, eth
m153	2-Methyl-1- butanol	CH ₃ CH ₂ CH(CH ₃)CH ₂ OH	88.15	1,388	0.816_4^{20}	1.4100^{20}	<-70	128	50	3 aq; misc alc, eth
m154	2-Methyl-2- butanol	CH ₃ CH ₂ C(CH ₃) ₂ OH	88.15	1, 388	0.8090^{20}	1.4050^{20}	-9.0	102.0	21	11 aq; misc alc, bz, chl, eth
m155	3-Methyl-1- butanol	(CH ₃) ₂ CHCH ₂ CH ₂ OH	88.15	1,392	0.8129415	1.408515	-117.2	132.0	45	2 aq; misc alc, bz, chl, eth, PE,
	outanoi									HOAc

α-Methylbenzyl alcohol, p112 N-Methylbenzylamine, b103 Methylbenzyl bromides, b368, b369 Methylbenzyl chlorides, c258, c259, c260 Methylbis(2-chloroethoxy)silane, b157 N-Methylbis(2-chloroethyl)amine, b159 Methyl bromide, b300 3-Methyl-1-buten-1-carboxylic acid, m349

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m156	3-Methyl-2-	(CH ₃) ₂ CHCH(OH)CH ₃	88.15	1, 391	0.817920	1.409620		111.5	26	2.8 aq; misc alc,
	butanol									eth
m157	3-Methyl-2-	(CH ₃) ₂ CHCOCH ₃	86.13	1,682	0.802_4^{20}	1.3890	92	94–95		misc alc, eth
	butanone									
m158	2-Methyl-1-butene	$CH_3CH_2C(CH_3) = CH_2$	70.14	1,211	0.6504_4^{20}	1.3777 ²⁰	-137.6	31.2		misc alc, eth
m159	2-Methyl-2-butene	$CH_3CH = C(CH_3)_2$	70.14	1,211	0.6620_4^{20}	1.3878^{20}	-133.8	38.6	-45	misc alc, eth; i aq
m160	3-Methyl-1-butene	$(CH_3)_2CHCH=CH_2$	70.14	$1^3,797$	0.6272_4^{20}	1.3638^{20}	-168.5	20.1		misc alc, eth
m161	(E)-2-Methyl-2- butenoic acid	CH ₃ CH=C(CH ₃)COOH	100.12	2,430	0.969	1.434281	64	198.5		s alc, eth; v s hot aq
m162	(Z)-2-Methyl-2- butenoic acid	CH ₃ CH=C(CH ₃)COOH	100.12	2, 428	0.98347	1.4437 ⁴⁷	45	185		s alc, eth; v s hot
m163	3-Methyl-2-butenoic acid	(CH ₃) ₂ C=CHCOOH	100.12	2, 432	1.006 ²⁴		69	194–195		s aq, alc, eth
m164	2-Methyl-3-buten- 2-ol	(CH ₃) ₂ C(OH)CH=CH ₂	86.13	1, 444	0.8672_{20}^{20}	1.4160 ²⁰	2.6	98–99	13	
m165	3-Methyl-3-buten- 1-ol	H ₂ C=C(CH ₃)CH ₂ CH ₂ OH	86.13		0.853	1.4337 ²⁰			36	
m166	2-Methyl-1-buten- 3-yne	H ₂ C=C(CH ₃)C≡CH	66.10	1 ¹ , 126		1.4140 ²⁰	-113	32	-6	
m167	<i>N</i> -Methylbutylamine	CH ₃ CH ₂ CH ₂ CH ₂ NHCH ₃	87.17	4, 157	0.736	1.3995^{20}	-75	91	<1	
m168	1-Methylbutylamine	CH ₃ CH ₂ CH ₂ CH-	87.17	4, 177	0.7384_4^{20}	1.4029^{20}		91	35	misc aq, alc, eth
		(CH ₃)NH ₂								_
m169	2-Methylbutylamine	CH ₃ CH ₂ CH(CH ₃)-	87.17	$4^3,342$	0.738	1.4116^{20}		94–97	3	
		CH ₂ NH ₂								
m170	3-Methylbutyl-	(CH ₃) ₂ CHCH ₂ CH ₂ OOC-	172.27	2, 312	0.8541^{25}	1.4100^{25}		194.0		misc alc, eth
	3-methylbutyrate	CH ₂ CH(CH ₃) ₂								
m171	3-Methyl-1-butyne	(CH ₃) ₂ CHC≡CH	68.12	1, 251	0.666_4^{20}	1.3740^{20}	-89.8	26.4		misc alc, eth
m172	2-Methyl-3-butyn-2-ol	(CH ₃) ₂ C(OH)C≡CH	84.12	1 ¹ , 235	0.8672_{20}^{20}	1.4209^{20}	2.6	104–105	25	misc aq, acet, bz

m173	2-Methylbutyr-	CH ₃ CH ₂ CH(CH ₃)CHO	86.13	11, 352	0.804	1.3919^{20}		90–92	4	
m174	aldehyde 3-Methylbutyr- aldehyde	(CH ₃) ₂ CHCH ₂ CHO	86.13	1,684	0.785_{20}^{20}	1.388220	-51	92–93	19	misc alc, eth; sl s
m175	Methyl butyrate	CH ₃ CH ₂ CH ₂ COOCH ₃	102.13	24, 786	0.898_4^{20}	1.3879^{20}	-85	102	14	1.4 aq; misc alc, eth
m176	2-Methylbutyric	CH ₃ CH ₂ CH(CH ₃)COOH	102.13	24, 888	0.936	1.4055^{20}		176.5	>112	Cui
m177	3-Methylbutyric acid	(CH ₃) ₂ CHCH ₂ COOH	102.13	2, 309	0.9308_4^{20}	1.4033^{20}	-30.0	176.5	70	4 aq; s alc, chl, eth
m178	3-Methylbutyro- nitrile	(CH ₃) ₂ CHCH ₂ CN	83.13	2^2 , 278	0.7925_4^{19}	1.3927 ²⁰	-101	129		misc alc, eth
m179	3-Methylbutyryl chloride	(CH ₃) ₂ CHCH ₂ COCl	120.58	2, 315	0.985_4^{20}	1.4161^{20}		115–117	18	d aq, alc; s eth
m180	l-(3-Methylbutyryl)- pyrrolidine		155.24		0.938	1.4710^{20}			104	
m181	Methyl carbamate	H ₂ NCOOCH ₃	75.07	3, 21	1.136456		52-54	177		220 aq; 73 alc; s eth
m182	Methyl chloro- acetate	CICH ₂ COOCH ₃	108.52	2, 197	1.238_{20}^{20}	1.4220^{20}	-33	130–132	57	i aq; misc alc, eth

(Z)-2-Methyl-2-butenedioic acid, c270 Methyl 2-buten-1-oate, m192 3-Methylbutyl acetate, i80 2-Methylbutylamine, a251 Methyl *tert*-butyl ether, b460 Methyl *tert*-butyl ketone, h72 2-Methylbutyl isovalerate, m170 Methyl caprate, m218 Methyl caproate, m265 Methyl carprylate, m329 Methyl carbazate, m271 Methyl carbitol, m66

4-Methylcatechol, d389 Methyl Cellosolve, m65 Methyl Cellosolve acetate, m68 β -Methylchalcone, d658 Methyl chlorocarbonate, m187

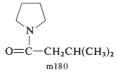


TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m183	Methyl 2-chloro-	CH ₃ COCH(Cl)COOCH ₃	150.56		1.236	1.4465 ²⁰	-32.7	137	71	
m184	acetoacetate Methyl <i>m</i> -chlorobenzoate	CIC ₆ H ₄ COOCH ₃	170.60	9, 338		1.4923 ²⁰	21	101 ^{12mm}		
m185	Methyl p-chloro- benzoate	ClC ₆ H ₄ COOCH ₃	170.60	9, 340	1.38220		44			s alc
m186	Methyl 4-chloro- butyrate	ClCH ₂ CH ₂ CH ₂ COOCH ₃	136.58	2, 278	1.126814	1.432120		176	59	v s eth; s alc, acet
m187	Methyl chloro- formate	CICOOCH ₃	94.50	3,9	1.223420	1.3865 ²⁰		71	<1	misc alc, bz, chl,
m188	Methyl 3-(chloro- formyl)propionate	CH ₃ OOCCH ₂ CH ₂ COCl	150.56	2^2 , 553	1.223	1.440220		65 ^{3mm}	73	
m189	Methyl 2-chloro- propionate	CH ₃ CH(Cl)COOCH ₃	122.55	2, 248	1.075	1.419320		132–133	36	s alc
m190	2-Methylcinnam- aldehyde	C ₆ H ₅ CH=C(CH ₃)CHO	146.19	7, 369	1.04747	1.6045 ²⁰		149 ^{27mm}	79	
m191	6-Methylcoumarin		160.17	17, 337			75–76	303 ^{725mm}		
m192	Methyl crotonate	CH ₃ CH=CHCOOCH ₃	100.12	2,410	0.9444_4^{20}	1.4242^{20}		121	4	v s alc, eth; i aq
m193	Methyl cyanoacetate	NCCH ₂ COOCH ₃	99.09	2, 584	1.1225^{25}	1.4166 ²⁵	-13.1	205.1	110	misc alc, eth
m194	Methylcyclohexane	$C_6H_{11}CH_3$	98.19	5, 29	0.7694^{20}	1.4231^{20}	-126.6	100.9	-3	
m195	Methyl cyclohexane- carboxylate	C ₆ H ₁₁ COOCH ₃	142.20	9 ¹ , 5	0.9954_4^{16}	1.4445 ²⁰		183	60	i aq; s alc, eth
m196	4-Methyl-1,2-cyclo- hexanedicarb-		168.19		1.162	1.4774 ²⁰				
m197	oxylic anhydride 1-Methylcyclo- hexanol	$C_6H_{10}(CH_3)OH$	114.19	6, 11	0.9251 ²⁵	1.4587 ²⁵	26	168	67	i aq; s bz, chl
m198	(Z)-2-Methylcyclo- hexanol	C ₆ H ₁₀ (CH ₃)OH	114.19	6 ² , 17	0.9340_4^{20}	1.4654 ²⁰	7	165	58	misc alc, eth

m199	(E)-2-Methylcyclo-	$C_6H_{10}(CH_3)OH$	114.19	6, 11	0.9247_4^{20}	1.4616^{20}	-4	165.5	58	misc alc; s eth
	hexanol				20	20	_			
m200	(Z)-3-Methylcyclo-	$C_6H_{10}(CH_3)OH$	114.19	6, 12	0.9155^{20}	1.4572^{20}	-6	94	62	misc alc, eth
201	hexanol				0.024.420	4 450020				
m201	(E)-3-Methylcyclo- hexanol	$C_6H_{10}(CH_3)OH$	114.19	6, 12	0.9214^{20}	1.4580^{20}	-1	84	62	
m202	(Z)-4-Methylcyclo-	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9122_4^{20}	1.4614^{20}		171	70	misc alc, eth
	hexanol									
m203	(E)-4-Methylcyclo-	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9118_4^{21}	1.4559^{20}		173–175	70	misc alc; s eth
	hexanol									
m204	2-Methylcyclo-	$CH_3C_6H_9(=O)$	112.17	7, 14	0.925_4^{20}	1.4478^{20}		162–163	46	i aq; s alc, eth
	hexanone									
m205	3-Methylcyclo-	$CH_3C_6H_9(=O)$	112.17	7, 15	0.9155_4^{20}	1.4460^{20}		168-169	51	i aq; s alc, eth
	hexanone									_
m206	4-Methylcyclo-	$CH_3C_6H_9(=O)$	112.17	7, 18	0.916_4^{20}	1.4455^{20}		169-171	40	i aq; s alc, eth
	hexanone									_
m207	1-Methyl-1-cyclo-		96.17	5, 66	0.809_4^{20}	1.4502^{20}	-121	111	-3	i aq; s alc, eth
	hexene									
m208	4-Methyl-1-cyclo-		96.17	5,67	0.799	1.4412^{20}	-115.5	102	-1	i aq; s alc, eth
	hexene									
m209	N-Methylcyclo-	C ₆ H ₁₁ NHCH ₃	113.20	12,6	0.868	1.4560^{20}		149	29	
	hexylamine	0 11 3		,						

Methyl chloroform, t226

(E)-2-Methylcrotonic acid, m161

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m210	3-Methylcyclo-	C ₆ H ₁₀ (CH ₃)NH ₂	113.20	12, 10	0.855	1.452520		150 ^{730mm}	22	
m211	hexylamine 4-Methylcyclo- hexylamine	C ₆ H ₁₀ (CH ₃)NH ₂	113.20	12, 12	0.855	1.4531 ²⁰		151–154	26	
m212	Methylcyclopenta- diene dimer		160.26		0.941	1.4976 ²⁰	-51	200	26	
m213 m214	Methylcyclopentane 3-Methyl-1,2-cyclo- pentanedione	C ₅ H ₉ CH ₃	84.16 112.13	5, 27 7 ¹ , 310	0.7487 ²⁰	1.4097 ²⁰	-142.4 105-107	71.8	-27	0.013 aq
m215	2-Methylcyclo- pentanone		98.15	7^2 , 13	0.9200_4^{20}	1.4347 ²⁰	-76	139–140		s aq; v s alc, eth
m216	3-Methyl-2-cyclo- penten-1-one		96.13	71,46	0.971	1.4780 ²⁰		74 ^{15mm}	65	
m217	2-Methylcyclo- propanecarboxylic acid		100.12	9,6	1.027	1.4395 ²⁰		191 ^{745mm}	87	
m218	Methyl decanoate	CH ₃ (CH ₂) ₈ COOCH ₃	186.30	2, 356			-18	223–224		i ag; misc alc, eth
m219	Methyl dichloro-	Cl ₂ CHCOOCH ₃	142.97	2, 203	1.380819	1.442120	-52	143	80	i aq; s alc
m220	Methyl 2,2-dichloro- 1-methylcyclopro- panecarboxylate		183.03		1.245	1.4639 ²⁰		74 ^{8mm}	74	
m221	Methyl 2,3-dichloro- propionate	ClCH ₂ CH(Cl)COOCH ₃	157.00	2 ¹ , 111	1.3282420	1.4447 ²⁰		92 ^{50mm}	42	s alc
m222	Methyldichloro- silane	CH ₃ SiHCl ₂	115.0		1.1047_4^{20}	1.422220	-93	41	-25	
m223	N-Methyldiethanol- amine	CH ₃ N(CH ₂ CH ₂ OH) ₂	119.16	4, 284	1.0377 ²⁰	1.4685 ²⁰		246–248	126	misc aq, alc

m224	O-Methyl-N,N'-	(CH ₃) ₂ CHNHC-	158.25		0.871	1.4358^{20}		50- 52 ^{0.1mm}	35	
m225	diisopropylurea Methyl 3,4-dimethoxybenzoate	(OCH_3) = $NCH(CH_3)_2$ $(CH_3O)_2C_6H_3COOCH_3$	196.20	10, 396			57–60	283		
m226	Methyl 4,5-dimeth- oxy-2-nitrobenz- oate	(CH ₃ O) ₂ C ₆ H ₂ (NO ₂)- COOCH ₃	241.20	10, 403			141–144			
m227	Methyl 2,2-di- methylpropionate	(CH ₃) ₃ CCOOCH ₃	116.16	2 ¹ , 139	0.873	1.3880 ²⁰		101–103	-1	misc alc, eth; sl s
m228	2-Methyl-3,5-di- nitrobenzoic acid	CH ₃ C ₆ H ₂ (NO ₂) ₂ COOH	226.15	9, 474			205–207			-
m229	N-Methyldioctyl- amine	$(C_8H_{17})_2NCH_3$	255.49	4 ³ , 381		1.4424 ²⁰	-30.1	165 ^{15mm}		
m230	N-Methyldiphenyl- amine	$(C_6H_5)_2NCH_3$	183.26	12, 180	1.048_4^{20}	1.6193 ²⁰	-7.6	135 ^{6mm}		i aq; s alc, eth
m231	Methyldiphenyl- silane	$(C_6H_5)_2Si(H)CH_3$	198.3		0.997_4^{20}	1.56920				
m232	N,N'-Methylenebis- acrylamide	H ₂ C=CHCONHCH ₂ NH- COCH=CH ₂	154.17				>300			
m233	2,2'-Methylenebis- (4-chlorophenol)	$CH_2[C_6H_3(Cl)OH]_2$	269.13				177–178			100 EtOH; 100 eth; s PE

Methyl 4,6-dimethyl-2-oxo-2*H*-pyran-5-carboxylate, m288

Methyldinitrophenols, d631, d633a Methyl enanthate, m261 Methylene bromide, d88

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m234	4,4'-Methylenebis- (<i>N</i> , <i>N</i> -dimethyl- aniline	CH ₂ [C ₆ H ₄ N(CH ₃) ₂] ₂	254.38	13, 239			90			
m235	4,4'-Methylenebis- (3-hydroxy-2- naphthoic acid	CH ₂ [C ₁₀ H ₅ (OH)COOH] ₂	388.38	10, 575			d>280			i aq, alc, eth, bz; sl s chl; s pyr
m236	1,1'-Methylenebis(3- methylpiperidine)	$CH_2(CH_3C_5H_9N)_2$	210.37		0.887	1.4734 ²⁰		160 ^{50mm}	110	
m237	Methylene blue		373.90	27, 393			190 d			4 aq; 1.3 alc; s chl
m238	4,4'-Methylenedi- aniline	$CH_2(C_6H_4NH_2)_2$	198.26	13, 238			92		221	•
m239	3,4-Methylenedi- oxybenzaldehyde		150.13	19, 115			37	264		0.2 aq; v s alc, eth
m240	1,2-Methylenedi- oxybenzene		122.12	19, 20	1.064	1.5398		173	55	
m241	3,4-Methylenedi- oxybenzoic acid		166.13	19, 269			229	subl 210		sl s aq, chl, alc, eth
m242	3,4-Methylenedi- oxybenzyl alcohol		152.14	19,67			53–55			
m243	3,4-Methylenedioxy- 6-propylbenzyldi- ethyleneglycol butyl ether		338.45		1.05	1.50 ²⁰		180 ^{1mm}	171	misc alc, bz, freons
m244	5-Methylene-2-nor- bornene		106.17		0.981	1.4819 ²⁰			4	
m245	Methylenesuccinic acid	H ₂ C=C(COOH)CH ₂ - COOH	130.10	2,760	1.573		162 d			8.2 aq; 20 alc; v s bz, chl, eth, PE
m246	N-Methylethylamine	CH ₃ CH ₂ NHCH ₃	59.11	$4^2,589$	0.690	1.3760		35	-12	v s aq, alc

m247	N-Methylethylenedi-	CH ₃ NHCH ₂ CH ₂ NH ₂	74.13	$4^{1},415$	0.841	1.4395^{20}		114–116	41	
	amine									
m248	N-Methylformamide	HCONHCH ₃	59.07	4, 58	0.9988^{25}	1.4300^{25}	-3.8	180–185	98	misc aq
m249	N-Methylformanilide	C ₆ H ₅ N(CH ₃)CHO	135.17	12, 234	1.095	1.5593^{20}	8-13	244	126	
m250	Methyl formate	HCOOCH ₃	60.05	2, 18	0.981515	1.346515	-99.0	31.5	-32	23 aq; misc alc
m251	5-Methylfuraldehyde		110.11	17, 289	1.1072_4^{18}	1.5263^{20}		187	72	s aq; v s alc; misc
										eth
m252	2-Methylfuran		82.10	17, 36	0.915_4^{20}	1.4332^{20}	-88	63-66	-26	0.3 aq
m253	Methyl furoate		126.11	18, 274	1.179^{20}	1.4862^{20}		181	73	s alc, eth; sl s aq
m254	Methylgermanium	CH ₃ GeBr ₃	327.35		2.6337_4^{20}	1.5770^{20}		168		
	tribromide									

Methylene bromochloride, b256 Methylene chloride, d190 4,4'-Methylenedianiline, d35 Methylene dimethyl ether, d441 Methylene iodide, d404 1,1'-Methylenedipiperidine, d695 β -Methylene- β -propiolactone, d422 (E)-3,6-endo-Methylene-1,2,3,6-tetrahydronaphthaloyl dichloride, n109 Methyl ethyl ketone, b393

Methyl fluoroform, t291 Methyl 2-furancarboxylate, m253 5-Methylfurfural, m251 α -Methyl-D-glucopyranoside, m256

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m255	N-Methyl-D-		195.22				128-129			100 aq; 1.2 alc
	glucamine									
m256	α-Methylglucoside		194.19	31, 179	1.46_4^{30}		168	200 ^{0.2mm}		63 aq; i alc, eth
m257	DL-2-Methyl-	NCCH ₂ CH ₂ CH(CH ₃)CN	108.14	2,656	0.950			125 ^{10mm}	126	
	glutaronitrile									
m258	N-Methylglycine	CH ₃ NHCH ₂ COOH	89.09	4, 345			d 212			42 aq; sl s alc
m259	Methyl glycolate	HOCH ₂ COOCH ₃	90.08	3, 236	1.168_4^{18}		74	151		s aq; misc alc, eth
m260	2-Methylheptane	CH ₃ (CH ₂) ₄ CH(CH ₃) ₂	114.23	1, 161	0.6978_4^{20}	1.3974^{20}	-109.0	117.7	4	s eth; sl s alc
m261	Methyl heptanoate	CH ₃ (CH ₂) ₅ COOCH ₃	144.22	2, 339	0.8815_4^{20}	1.4115^{20}	-55.8	173.8	52	s alc, eth; sl s aq
m262	6-Methyl-5-hepten-	(CH ₃) ₂ C=CHCH ₂ CH ₂ -	126.20	$1^2,797$	0.855_4^{16}	1.4392^{20}	-67	73 ^{18mm}	50	misc alc, eth
	2-one	COCH ₃								
m263	Methyl hexa-	CH ₃ (CH ₂) ₄ COOCH ₃	270.46	2, 372			28	196 ^{15mm}		s alc, chl, eth
	decanoate									
m264	2-Methylhexane	CH ₃ (CH ₂) ₃ CH(CH ₃) ₂	100.21	1, 156	0.6786^{20}	1.3849^{20}	-118.3	90.1	-3	s alc; misc eth
m265	Methyl hexanoate	CH ₃ (CH ₂) ₄ COOCH ₃	130.19	2, 323	0.9038_4^0	1.4038^{23}	-71	151	54	v s alc, eth
m266	5-Methyl-2-hexanol	(CH ₃) ₂ CHCH ₂ CH ₂ -	116.20	1,416	0.814_4^{20}	1.4176^{20}		150	46	s alc, eth; i aq
		CH(OH)CH ₃								
m267	5-Methyl-2-hexanone	(CH ₃) ₂ CHCH ₂ CH ₂ -	114.19	$1^2,756$	0.888_4^{20}	1.4062^{20}		141	41	0.5 aq; misc alc,
		COCH ₃								eth
m268	5-Methyl-3-hexen-	(CH ₃) ₂ CHCH=CHCOCH ₃	112.17			1.4400^{20}				
	2-one									
m268a	1-Methylhexylamine	H(CH ₂) ₅ CH(NH ₂)CH ₃	115.22	4, 194	0.7665^{18}	1.4175^{20}		144	54	sl s aq; s alc, eth
m269	1-Methylhydantoin		114.10	24, 244			157	subl		s aq, alc; 3 eth
m270	Methylhydrazine	CH ₃ NHNH ₂	46.07	$4^2,957$	0.866	1.4235^{20}	-52.4	87.5	21	misc aq, alc; s PE
m271	Methyl hydrazino-	H ₂ NNHCOOCH ₃	90.08	3 ¹ , 46			70-73	108 ^{12mm}		
	carboxylate									
m272	Methyl hydrogen	HOOCCH ₂ CH ₂ CH ₂	146.14	2^2 , 565	1.169	1.4381^{20}		151 ^{10mm}	>112	
	glutarate	COOCH ₃								
	I	ı		ı	1	ı	ı	1	I	I

m273	Methyl hydrogen hexanedioate	HOOC(CH ₂) ₄ COOCH ₃	160.17	2,652	1.081	1.4401^{20}	8–9	162 ^{10mm}	>112	s alc
m274	Methyl hydrogen succinate	HOOCCH ₂ CH ₂ COOCH ₃	132.12	2, 608			56–59	151 ^{20mm}		v s aq, alc, eth
m275	Methyl hydro- peroxide	CH ₃ OOH	48.04	1 ² , 270	1.99745	1.364215		38 ^{65mm}		misc aq, alc, eth;
m276	Methylhydroquinone		124.14	6, 874			125-128			
m277	Methyl 4-hydroxy- benzoate	HOC ₆ H ₄ COOCH ₃	152.15	10, 158			126–128	270 d		v s alc, eth, acet
m278	Methyl 2-hydroxy- isobutyrate	(CH ₃) ₂ C(OH)COOCH ₃	118.13	$3^2, 223$	1.023	1.4112^{20}		137	42	v s aq, alc
m279	Methyl 4-hydroxy- phenylacetate	HOC ₆ H ₄ CH ₂ COOCH ₃	166.18	10, 191			57-60	162- 163 ^{5mm}		
m280	1-Methylimidazole		82.11	23, 46	1.030	1.4970^{20}	-60	198	92	misc aq
m281	2-Methylimidazole		82.11	23, 65			143	268		_
m282	4-Methylimidazole		82.11	23, 69			46–48	263	>112	

N-Methylguanidine acetic acid, c277 4-Methylhexahydrophthalic anhydride, m196 Methyl hydroxyacetate, m259 Methyl 4-hydroxy-3-methoxybenzoate, m445 Methyl 2-hydroxypropionate, m291 2,2'-Methyliminodiethanol, m223 2,2'-Methyliminobis(acetaldehyde diethyl acetal), b169

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m283	2-Methyl-1 <i>H</i> -indole		131.18	20, 311	1.07420		58-60	273		v s alc, eth; s hot
m284 m285	3-Methyl-1 <i>H</i> -indole <i>N</i> -Methylisatoic anhydride		131.18 177.16	20, 315 27, 265			95 165 d	266		aq s hot aq, alc, bz
m286	Methyl isobutyrate	(CH ₃) ₂ CHCOOCH ₃	102.13	2, 290	0.89120	1.3840^{20}	-84	93	<1	misc alc, eth; sl s
m287 m288	Methyl isocyanate Methyl isodehyd- acetate	CH ₃ NCO	57.05 182.18	4, 77 18, 410	0.967	1.3695 ²⁰	-17 60-63	37–39 167 ^{14mm}	-18	s aq
m289	Methyl isothio- cyanate	CH₃NCS	73.12	4,77	1.069	1.5258 ³⁷	35–36	119	32	v s alc, eth; sl s aq
m290 m291	5-Methylisoxazole Methyl lactate	CH ₃ CH(OH)COOCH ₃	83.09 104.10	27, 16 3, 280	$ \begin{array}{c} 1.018 \\ 1.088_4^{20} \end{array} $	$1.4386^{20} \\ 1.4131^{20}$	~66	122 144.8	30 52	misc aq(d), alc,
m292 m293	Methyl mandelate Methyl mercapto- acetate	C ₆ H ₅ CH(OH)COOCH ₃ HSCH ₂ COOCH ₃	166.18 106.14	10, 202	1.1756 ²⁰ 1.187	1.4657 ²⁰	51–54	135 ^{12mm} 43 ^{10mm}	30	s aq, alc, bz, chl s alc, eth
m294	Methyl 3-mercapto- propionate	HSCH ₂ CH ₂ COOCH ₃	120.17	$3^2, 214$	1.085	1.4640^{20}		55 ^{14mm}	60	
m295	Methylmercury chloride	CH₃HgCl	251.10		4.06^{25}		170			
m296	Methyl methacrylate	$H_2C = C(CH_3)COOCH_3$	100.12	$2^2,398$	0.9433 ²⁰	1.4146^{20}	-48.2	100.3	10	1.6 aq; s ketones, esters, CCl ₄
m297	Methyl methane- sulfonate	CH ₃ SO ₂ OCH ₃	110.13	4, 4	1.2943420	1.4138^{20}		202–203	104	20 aq; 100 DMF
m298	Methyl methoxy- acetate	CH ₃ OCH ₂ COOCH ₃	104.11	3, 236	1.0511420	1.3964 ²⁰		130	35	v s alc, eth; sl s aq

m299	Methyl 1-methoxybi-		196.25		1.086	1.4886^{20}	105 ^{17mm}	103	
	cyclo[2.2.2]oct-								
	5-ene-2-carboxylate								
m300	Methyl 4-methoxy-	CH ₃ OC ₆ H ₄ CH ₂ COOCH ₃	180.20	10, 191	1.135	1.5165^{20}	158 ^{19mm}	36	
	phenylacetate								
m301	1-Methyl-4-(methyl-		128.22		0.882	1.4672^{20}		55	
	amino)piperidine								
m302	Methyl 3-methyl-	(CH ₃) ₂ CHCH ₂ COOCH ₃	116.16	2^2 , 274	0.881_4^{20}	1.3800^{25}	116-117		sl s aq; misc alc,
	butyrate								eth
m303	2-Methyl-6-methyl-	$C_2H_5C(=CH_2)(CH_2)_3$ -	156.27		0.784	1.443120	84 ^{10mm}	76	
	ene-2-octanol	C(CH ₃) ₂ OH							

Methyl iodide, i40 Methyl isoamyl ketone, m267 Methyl isobutenyl ketone, m350 Methyl isobutyl ketone, m346 Methyl isonicotinate, m402 Methyl isopentyl ketone, m267

Methyl isovalerate, m302 2-Methyllactic acid, h127 Methyl linoleate, m325 Methyl mercaptan, m33 Methylmercaptoanilines, m422, m423 4-Methylmercaptobenzaldehyde, m424

Methylmercaptophenols, m431a, m429 7-Methyl-3-methylene-1,6-octadiene, m453 1-Methyl-4-(1-methylethenyl)cyclohexane, d649 5-Methyl-2-(1-methylethyl)cyclohexanol, m12 5-Methyl-2-(1-methylethyl)cyclohexanone, m13

m290

m288

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m304	Methyl 2-methyl-		140.14		1.116	1.473020		75 ^{20mm}	63	
m305	3-furancarboxylate Methyl S-methyl- thiomethyl sulfoxide	CH ₃ S(=O)CH ₂ SCH ₃	124.22		1.191	1.5487 ²⁰		95 ^{2.5mm}	>112	
m306	Methyl 3-(methyl-thio)propionate	CH ₃ SCH ₂ CH ₂ COOCH ₃	134.20		1.077	1.4650 ²⁰		75 ^{13mm}	72	
m307	N-Methylmorpholine		101.15	27,6	0.920	1.4349^{20}	-66	116	23	s aq, alc, eth
m308	1-Methylnaphthalene	$C_{10}H_7CH_3$	142.20	5, 566	1.025_4^{14}	1.6159^{20}	-30.5	244.7	82	v s alc, eth
m309	2-Methylnaphthalene	$C_{10}H_7CH_3$	142.20	5, 567	1.029_4^{20}	1.602640	34.6	241.4		v s alc, eth
m310	2-Methyl-1,4- naphthoquinone		172.18	$7^2,656$			105–107			1.4 alc; 10 bz; s chl
m311	Methyl 1-naphthyl ketone	C ₁₀ H ₇ COCH ₃	170.21	7, 401	1.13364	1.6284 ²⁰	12	296–298		s alc, eth; i aq
m312	Methyl 2-naphthyl ketone	C ₁₀ H ₇ COCH ₃	170.21	7, 402			53–55	300–301		sl s alc; s CS ₂
m313	Methyl nitrate	CH ₃ ONO ₂	77.04	1, 284	1.2075_4^{20}	1.3748 ²⁰	-83.0	64 explodes		sl s aq; s alc, eth
m314	Methyl nitrate	CH ₃ ONO	61.04	1, 284	0.991 (liquid)			-17.35		s alc, eth
m315	2-Methyl-4-nitro- aniline	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 846	1.586 ₄ ¹⁴⁰		131–133			v s alc; s bz
m316	2-Methyl-5-nitro-	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 844			104–107			s alc, acet, eth
m317	4-Methyl-2-nitro- aniline	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 100			115–116			v s alc; s eth
m318	Methyl 2-nitro- benzoate	O ₂ NC ₆ H ₄ COOCH ₃	181.15	9, 372	1.280	1.5350 ²⁰	-13	106 ^{0.1mm}	>112	s alc, eth

m319	2-Methyl-3-nitro-	CH C H (NO)COOH	181.15	9,471	I		182–184	1		
111319	benzoic acid	CH ₃ C ₆ H ₃ (NO ₂)COOH	161.13	9,4/1			102-104			
220		CH C H (NO)COOH	101 15	0.502			187–190			
m320	4-Methyl-3-nitro-	CH ₃ C ₆ H ₃ (NO ₂)COOH	181.15	9,502			187-190			
	benzoic acid									
m321	5-Methyl-2-nitro-	CH ₃ C ₆ H ₃ (NO ₂)-COOH	181.15	9, 482			134–136			
	benzoic acid									
m322	2-Methyl-5-nitro-		127.10	$23^1, 23$			252-254			
	imidazole									
m323	3-Methyl-2-nitro-	CH ₃ C ₆ H ₃ (NO ₂)OH	153.14	6, 385			35-39			
	phenol	_								
m324	4-Methyl-2-nitro-	CH ₃ C ₆ H ₃ (NO ₂)OH	153.14	6,412	1.240^{20}_{4}	1.574^{40}	32-35	125 ^{22mm}		v s alc, eth
	phenol	3 0 3(2)		,	-					
m325	Methyl 9,12-octa-	CH ₃ (CH ₂) ₄ CH=CHCH ₂ -	294.46		0.8886^{18}_{4}	1.4593^{25}	-35	212 ^{16mm}		misc DMF
	decadienoate	$CH = CH(CH_2)_7 COOCH_3$								
m326	Methyl octa-	CH ₃ (CH ₂) ₁₆ COOCH ₃	298.51	2,379			38-39	215 ^{15mm}	>112	s alc, eth
	decanoate	2.13								
m327	Methyl cis-9-octa-	$CH_3(CH_2)_7CH = CH$	296.50	2,467	0.879^{18}_{4}	1.4521^{20}	19.9	168 ^{2mm}		misc abs alc, eth
	decenoate	(CH ₂) ₇ COOCH ₃			-					
m328	Methyloctadecyldi-	C ₁₈ H ₃₇ Si(CH ₃)Cl ₂	367.5		0.930_4^{20}			185 ^{2.5mm}		
		10 37 \ 37 - 2								
111328	chlorosilane	$C_{18}\Pi_{37}$ 31($C\Pi_3$) Cl_2	307.3		0.9304			163		

Methyl 2-methyllactate, m278 Methyl methyl-2-propenoate, m296 Methyl methylsulfinylmethyl sulfide, m305 Methyl myristate, m413 Methyl nicotinate, m404 4-Methyl-3-nitroanisole, m85 Methyl 6-nitrovertrate, m226 Methyl nonyl ketone, u5 Methyl oleate, m327

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m329 m330	Methyl octanoate Methyloctyldichloro- silane	CH ₃ (CH ₂) ₆ COOCH ₃ C ₈ H ₁₇ Si(CH ₃)Cl ₂	158.24 227.3	2, 348	$0.8775_4^{20} \\ 0.976_4^{20}$	$1.4160^{25} 1.444^{20}$	-40	192.9 94 ^{6mm}		v s alc, eth; i aq
m331	3-Methyl-2-oxazo- lidinone		101.11		1.170	1.4541 ²⁰	15	87– 90 ^{1mm}	>112	
m332	2-Methyl-2-oxazo- line		85.11	27, 11	1.005	1.4340^{20}		110	20	
m333	Methyl 2-oxocyclo- pentanecarboxylate		142.15	10, 597	1.145	1.4560^{20}		105 ^{19mm}	>112	
m334	Methyl 2-oxo- propionate	CH ₃ C(=0)COOCH ₃	102.09	3, 616	1.130	1.4065 ²⁰		134–137	39	misc alc, eth; sl s
m335	Methyl 2-oxo-1- pyrrolidineacetate		157.17		1.131	1.4719^{20}			110	•
m336	2-Methylpentane	CH ₃ CH ₂ CH ₂ CH(CH ₃) ₂	86.18	1, 148	0.6532^{20}	$1.3725^{20} \\ 1.3765^{20}$	-153.7 < -50	60.3	-23 -6	
m337	3-Methylpentane	(CH ₃ CH ₂) ₂ CHCH ₃	86.18	1, 149	0.6643 ²⁰		glass	03.3	-6	
m338	2-Methyl-2,4- pentanediol	(CH ₃) ₂ C(OH)CH ₂ - CH(OH)CH ₂	118.18	1, 486	0.9216_4^{20}	1.4270^{20}	<-50 glass	198.3	101	misc aq
m339	4-Methylpentane-	(CH ₃) ₂ CHCH ₂ CH ₂ CN	97.16	2^2 , 290	0.8035_4^{20}	1.4061^{20}	-51.1	153.5		s alc; misc eth
m340	Methyl pentanoate	CH ₃ (CH ₂) ₃ COOCH ₃	116.16	2, 301	0.875	1.3962^{20}		128	22	sl s aq; misc alc, eth
m341	2-Methylpentanoic acid	CH ₃ CH ₂ CH ₂ CH(CH ₃)- COOH	116.16	$2^2, 288$	0.9242_{20}^{20}	1.4135^{20}	-85 glass	196.4	107	1.3 aq
m342	3-Methylpentanoic acid	CH ₃ CH ₂ CH(CH ₃)- CH ₂ COOH	116.16	2, 331	0.926220	1.4159^{20}	-42	196–198	85	s alc, eth
m343	2-Methyl-1-pentanol	CH ₂ COOH CH ₃ CH ₂ CH ₂ CH(CH ₃)- CH ₂ OH	102.18	1,409	0.824220	1.4190 ²⁰		148.0	50	s alc, eth

m344	3-Methyl-3-pentanol	(CH ₃ CH ₂) ₂ C(CH ₃)OH	102.18	1,411	0.828120	1.4186^{20}	<-38	122.4	46	misc alc, eth; sl s
2.45	434 4 10 4 1	(CH) CHCH	102.10	1 410	0.000020	1 411020	00	121.7	41	aq
m345	4-Methyl-2-pentanol	(CH ₃) ₂ CHCH ₂ - CH(OH)CH ₂	102.18	1.410	0.8080^{20}	1.4112^{20}	-90	131.7	41	1.6 aq
m346	4-Methyl-2-penta- none	(CH ₃) ₂ CHCH ₂ COCH ₃	100.16	1,691	0.8006_4^{20}	1.3958 ²⁰	-83.5	115.7	13	1.7 aq; misc alc, bz, eth
m347	2-Methyl-1-pentene	$CH_3CH_2CH_2$ - $C(CH_3)$ = CH_3	84.16	11,90	0.6799_4^{20}	1.3920^{20}	-135.7	62.1	-26	s alc
m348	2-Methyl-2-pentene	$CH_3CH_2CH = C(CH_3)_2$	84.16	1, 217	0.6865_4^{20}	1.4003^{20}	-135.1	67.3	-23	s alc
m349	4-Methyl-2-pentenoic acid	(CH ₃) ₂ CHCH= CHCHCOOH	114.14	$2^2,406$	0.9529	1.4489	35	115 ^{20mm}	46	i aq; v s alc
m350	4-Methyl-3-penten- 2-one	$(CH_3)_2C$ = $CHCOCH_3$	98.15	1,736	0.854 420	1.4458^{20}	-42	129.5	30	3.1 aq
m350a	1-Methylpentylamine	CH ₃ (CH ₂) ₃ - CH(NH ₂)CH ₂	101.19	4, 190	0.767_4^{20}		-19	116–118	13	s aq, alc, PE
m351	4-Methyl-1-pentyne	(CH ₃) ₂ CHCH ₂ C≡CH	82.15		0.7041_4^{20}	1.3930^{20}	-104.8	61.2		
m352	3-Methyl-1-pentyn- 3-ol	$CH_3CH_2C(CH_3)(OH)$ - $C \equiv CH$	98.15	1 ² , 506	0.8688_4^{20}	1.4318^{20}	-30.6	121–122	38	13 aq; misc bz, acet, PE, EtAc;
m353	Methyl-(2-phen- ethyl)dichloro-	C ₆ H ₅ CH ₂ CH ₂ Si(CH ₃)Cl ₂	219.2		1.11120	1.510^{20}		99 ^{6mm}		s eth
	silane									

o-Methylolphenol, h105 2-Methyloxacyclopropane, p227 Methyl oxirane, p227 Methyl palmitate, m263 Methyl pentyl ketone, h15

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m354	(1-Methylphenethyl)- trichlorosilane	C ₆ H ₅ CH(CH ₃)CH ₂ SiCl ₃	253.6		1.226420	1.515 ²⁰		116 ^{10mm}		
m355	N-(4-Methylphenyl)- acetamide	CH ₃ C ₆ H ₄ NHCOCH ₃	149.19	$12^2,501$	1.21215		153	307		s alc, EtAc, HOAc
m356	Methyl phenylacetate	C ₆ H ₅ CH ₂ COOCH ₃	150.18	9, 434	1.044	1.5075^{20}		215	90	i aq; misc alc, eth
m357	Methylphenylchloro- silane	C ₆ H ₅ (CH ₃)Si(H)Cl	156.7		1.1054_4^{20}	1.571 ²⁰		113 ^{100mm}		
m358	Methylphenyldi- chlorosilane	C ₆ H ₅ Si(CH ₃)Cl ₂	191.1		1.187_4^{20}			205–206		
m359	<i>p</i> -(1-Methyl-2-phenylethyl)phenol	C ₆ H ₅ CH ₂ CH(CH ₃)- C ₆ H ₄ OH	212.29				73	335		
m360	1-Methyl-1-phenyl- hydrazine	$C_6H_5N(CH_3)NH_2$	122.17	15, 117	1.038422	1.5834 ²⁰		118 ^{21mm}	96	misc alc, bz, chl,
m361	1-Methyl-3-phenyl- propyl acetate	C ₆ H ₅ CH ₂ CH ₂ CH(CH ₃)- OOCCH ₃	192.26	61, 258	0.991			74 ^{0.05mm}	>112	
m362	3-Methyl-1-phenyl- 2-pyrazolin-5-one	,	174.20	24, 20			130	287 ^{265mm}		
m363	Methylphenylsilane	C ₆ H ₅ Si(CH ₃)H ₂	122.1		0.889_4^{20}	1.506^{20}		139-240		
m364	Methyl phenyl sulfide	C ₆ H ₅ SCH ₃	124.21	6, 297	1.058	1.5852 ²⁰	-15	188		i aq; s alc
m365	N-Methylpiperazine		100.17		0.903	1.4655^{20}		138	42	v s aq, alc, eth
m366	2-Methylpiperazine		100.17	23, 17			65–67	155.6	22	78 aq; 37 acet; 32 bz
m367	4-Methyl-1-piper- azinepropanol		158.25	23³, 123		1.4835^{20}	28–30	120- 121 ^{9mm}		
m368	N-Methylpiperidine	$C_5H_{10}N$ — CH_3	99.19	20, 19	0.816	1.4378^{20}		106–107	<1	v s aq; misc alc,
m369	2-Methylpiperidine	CH ₃ C ₅ H ₉ NH	99.19	20, 95	0.844	1.4459 ²⁰	-5	119	8	v s aq; misc alc, eth

m370	3-Methylpiperidine	CH ₃ C ₅ H ₉ NH	99.19	20, 100	0.845	1.4470^{20}		126	<1	v s aq
m371	4-Methylpiperidine	CH ₃ C ₅ H ₉ NH	99.19	20, 101	0.838	1.4458^{20}		124	7	v s aq
m372	1-Methyl-3-piper- idinemethanol		129.20	21 ² , 8	1.013	1.4772 ²⁰		140–145	94	_
m373	1-Methyl-4-piper- idone		113.16	21 ² , 215	0.920	1.4614 ²⁰			60	
m374	2-Methylpropanal	(CH ₃) ₂ CHCHO	72.11	1,671	0.7891 ²⁰	1.3727 ²⁰	-65	64.1		9 aq; misc alc, bz, chl, eth
m375	2-Methylpropane	(CH ₃) ₃ CH	58.12	1, 124	0.557 ²⁰		-159.6	-11.7		13 mL aq; 1320 mL alc; 2890 mL eth
m376	N-Methyl-1,3- propanediamine	H ₂ NCH ₂ CH ₂ CH ₂ NHCH ₃	88.15	4 ¹ , 419	0.844	1.4468 ²⁰		139–141	35	
m377	2-Methyl-1,2- propanediamine	(CH ₃) ₂ C(NH ₂)CH ₂ NH ₂	88.15	4, 266	0.841	1.4410^{20}			23	
m378	1-Methyl-1-propane- thiol	CH ₃ CH ₂ CH(SH)CH ₃	90.19	1,373	0.8246_4^{25}	1.4338 ²⁵	-165	84–85	21	sl s aq; v s alc, eth

Methylphenols, c279, c280, c281 Methyl-*m*-phenylene diisocyanate, t172 Methyl phenyl ether, m48 Methyl phenyl ketone, a31 2-Methyl-2-phenylpropane, b425 Methyl γ -picolinate, m402 Methylpiperidinol, h144 Methyl pivalate, m227 1-Methyl-1-propanethiol, b389 Methyl propargyl ether, m396

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m379	2-Methyl-1-propane- thiol	(CH ₃) ₂ CHCH ₂ SH	90.19	1, 378	0.8357_4^{20}	1.4396 ²⁰	-79	88.5	-9	v s alc, eth
m380	2-Methyl-2-propane- thiol	(CH ₃) ₃ CSH	90.19	1, 383	0.7943425	1.4198 ²⁵	1.1	64.2	-26	i aq
m381	2-Methyl-1-propanol	(CH ₃) ₂ CHCH ₂ OH	74.12	1, 373	0.8016^{20}	1.3958 ²⁰	-108	107.9	27	10 aq; misc alc, eth
m382	2-Methyl-2-propanol	(CH ₃) ₃ COH	74.12	1,379	0.7858_4^{20}	1.3877^{20}	25.8	82.4	15	misc aq, alc, eth
m383	2-Methylpropene	$(CH_3)_2C=CH_2$	56.10	1, 207	0.6266_4^{-14}	þ	-140.4	-6.9		v s alc, eth
m384	2-Methyl-2-propene- 1-sulfonic acid, Na salt	H ₂ C=C(CH ₃)CH ₂ SO ₃ ⁻ Na ⁺	158.15				>300			
m385	2-Methyl-2-propen- 1-ol	H ₂ C=C(CH ₃)CH ₂ OH	72.11	1,443	0.857	1.4250^{20}		113–115	33	
m386	4-Methyl-2-(2-propenyl)phenol	$CH_3C_6H_3$ - $(CH_2CH=CH_2)OH$	148.21	61, 287	0.980	1.5385 ²⁰		238	101	
m387	6-Methyl-2-(2-propenyl)phenol	$CH_3C_6H_3$ - $(CH_2CH=CH_2)OH$	148.21	6 ¹ , 287	0.992	1.5381 ²⁰		231–233	94	
m388	N-Methylpropion- amide	CH ₃ CH ₂ CONHCH ₃	87.12		0.9305 ²⁵	1.4345 ²⁵	-30.9	148		
m389	Methyl propionate	CH ₃ CH ₂ COOCH ₃	88.11	2, 239	0.915_4^{20}	1.3770^{20}	-88	79.7	-2	6 aq; misc alc, eth
m390	2-Methylpropionic acid	(CH ₃) ₂ CHCOOH	88.11	2, 288	0.950_4^{20}	1.3930 ²⁰	-46.1	154.7	55	23 aq; misc alc, chl, eth
m391	4'-Methylpropio- phenone	CH ₃ C ₆ H ₄ COCH ₂ CH ₃	148.21	7, 317	0.993	1.5280 ²⁰	7.2	239	96	
m392	Methylpropyldi- chlorosilane	CH ₃ CH ₂ CH ₂ Si(CH ₃)Cl ₂	157.1		1.04_4^{25}	1.425 ²⁵		125		
m393	Methyl propyl ether	CH ₃ CH ₂ CH ₂ OCH ₃	74.12	1, 354	0.73820			39.1		sl s aq; misc alc, eth

m394	2-Methyl-2-propyl- 1,3-propanediol	$C_3H_7C(CH_3)(CH_2OH)_2$	132.20	1 ¹ , 254			53–55	230		
m395	Methyl propyl sulfide	CH ₃ SCH ₂ CH ₂ CH ₃	90.18	1 ³ , 1432	0.8424 ²⁰	1.4442^{20}	-113.0	95.5		s aq
m396	Methyl 2-propynyl ether	CH₃OCH₂C≡CH	70.09	1,454	0.830	1.3961^{20}		61–62	<1	
m397	2-Methylpyrazine		94.12	23, 94	1.030	1.5042^{20}	-29	135	50	v s ag, alc, eth
m398	2-Methylpyridine	CH ₃ C ₅ H ₄ N	93.13	20, 234	0.950_4^{15}	1.5010^{20}	-67	128-129	26	v s aq; s alc, eth
m399	3-Methylpyridine	CH ₃ C ₅ H ₄ N	93.13	20, 239	0.961_4^{15}	1.5068^{20}	-18.3	143.5	36	s aq, alc, eth
m400	4-Methylpyridine	CH ₃ C ₅ H ₄ N	93.13	20, 240	0.957_4^{15}	1.5058	3.8	143-145	56	s aq, alc, eth
m401	Methyl 3-pyridine-	(C ₅ H ₄ N)COOCH ₃	137.14	22, 39			39	209		s aq, alc, bz
	carboxylate									
m402	Methyl 4-pyridine-	(C ₅ H ₄ N)COOCH ₃	137.14	22, 46	1.001	1.5122^{20}	8.5	207-209	82	
	carboxylate									
m403	1-Methyl-2-pyridone		109.13	21, 268	1.112	1.5690^{20}	7	250 ^{740mm}		
m404	N-Methylpyrrole		81.2	20, 163	0.914	1.4875^{20}	-57	113	15	i aq; misc alc, eth

- 2-Methylpropenenitrile, m27
- 2-Methylpropenoic acid, m26
- 2-Methylpropionaldehyde, i73
- 2-Methylpropionamide, i74
- 2-Methylpropionic acid, i75
- 2-Methylpropionitrile, i76

- 1-Methylpropyl acetate, b413
- 2-Methylpropyl acetate, i62
- 2-Methyl-2-propylamine, b418
- 2-Methylpropylamine, i63
- (1-Methylpropyl)benzene, b424
- (2-Methylpropyl)benzene, i64

- 2-Methylpropyl formate, i66
- 2-Methylpropyl lactate, i68
- Methyl propyl ketone, p41
- 2-Methylpropyl 2-methylpropanoate, i67
- Methyl pyruvate, m334
- Methyl pyridyl ketones, a53, a54, a55

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m405 m406	N-Methylpyrrolidine N-Methyl-2-pyrrolidinone		85.15 99.13	20, 4 21 ² , 213	$0.819_4^{20} \\ 1.0279^{25}$	1.4247 ²⁰ 1.4680 ²⁵	-24.4	80–81 202	-21 95	misc aq, eth misc aq, alc, bz, eth
m407	2-Methylquinoline		143.19	20, 387	1.058	1.6108^{20}	-2	248	79	i aq; s chl, eth
m408	4-Methylquinoline		143.19	20, 395	1.0826_4^{20}	1.6200^{20}	9–10	261-263	>112	misc alc, bz, eth
m409	2-Methylquinoxaline		144.18	231, 44	1.118	1.6156^{20}	180-181	245–247	107	misc aq
m410	Methyl salicylate	HOC ₆ H ₄ COOCH ₃	152.15	10, 70	1.1831 ²⁰	1.5240 ²⁰	-8.6	223.0	110	0.7 aq; s chl, eth; misc alc, HOAc
m411	α -Methylstyrene	$C_6H_5C(CH_3)=CH_2$	118.18	5, 484	0.909	1.5375^{20}	-23.2	165.5	45	
m412	Methylsuccinic acid	HOOCCH ₂ CH(CH ₃)COOH	132.12	2,636	1.411	1.4303	110-112	d		66 aq; v s alc, eth
m413	Methyl tetra- decanoate	CH ₃ (CH ₂) ₁₂ COOCH ₃	242.40	$2^2,326$	0.855	1.436220	18.4	323	>112	misc alc, bz, eth
m414	2-Methyl-3,3,4,4- tetrafluoro-2- butanol	HCF ₂ CF ₂ C(CH ₃) ₂ OH	160.11		1.282	1.3524 ²⁰		117	73	
m415	2-Methyltetra- hydrofuran		86.13	17, 12	0.860	1.4056 ²⁰		78–80	-11	
m416	1-Methyl-1,2,3,6-		97.16		0.837	1.4570 ²⁰		113–114	8	
m417	tetrahydropyridine 3-Methyltetrahydro- thiophene-1,1- dioxide		134.20		1.191	1.4772 ²⁰		276	>112	
m418	4-Methyl-5-thiazole- ethanol		143.21		1.196	1.5508 ²⁰		135 ^{7mm}		
m419	2-Methyl-2- thiazoline		101.17	27, 13	1.067	1.5200^{20}	-101	145	37	
m420	Methyl thioacetate	CH ₂ COSCH ₂	90.14			1.4628		98	10	s alc, eth
m421	(Methylthio)aceto- nitrile	CH ₃ SCH ₂ CN	87.14		1.039	1.4826 ²⁰		63 ^{15mm}	67	3 415, 541

m422	2-(Methylthio)-	CH ₃ SC ₆ H ₄ NH ₂	139.22	13, 399	1.111	1.6239^{20}		234	>112	
m423	aniline 3-(Methylthio)-	CH ₃ SC ₆ H ₄ NH ₂	139.22	13¹, 141	1.130	1.6423 ²⁰		165 ^{16mm}	>112	
42.4	aniline	CH CC H CHO	152.22	8 ¹ , 533	1.144	1.6452 ²⁰		90 ^{1mm}		
m424	4-(Methylthio)- benzaldehyde	CH ₃ SC ₆ H ₄ CHO	132.22	8,333	1.144	1.0432		90		
m425	3-(Methylthio)-2- butanone	CH ₃ CH(SCH ₃)COCH ₃	118.20	14, 3993	0.975	1.4710^{20}		50- 54 ^{20mm}	44	
m426	Methyl thiocyanate	CH₃SCN	73.12	3, 175	1.068^{20}	1.4697^{20}	-51	130-133	38	i aq; misc alc, eth
m427	3-Methylthiophene		98.17	17, 38	1.016	1.5180^{20}	-69.0	115.4	11	i aq; misc alc, eth
m428	5-Methyl-2-thio-		126.18	17 ¹ , 151	1.170	1.5825^{20}		114 ^{25mm}	87	
	phenecarbaldehyde									
m429	4-(S-Methylthio)-	CH ₃ SC ₆ H ₄ OH	140.20	6 ¹ , 419			83-85	153-		
	phenol							156 ^{20mm}		

1-Methyl-2-(3-pyridyl)pyrrolidine, n20 Methylresorcinol, d390 Methylsalicyclic acids, h137, h138 Methyl stearate, m326

Methylsuccinyl chloride, m188 methylsulfonic acid, m30 Methyl theobromine, c1 3-Methyl-2-thiabutane, i104

Methyl thienyl ketone, a57 Methyl thioglycolate, m293

m428

 CH_3

Ò.

m417

CH₃

m419

m427

m418

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m430	3-Methylthio-1,2- propanediol	CH ₃ SCH ₂ CH(OH)CH ₂ OH	122.19		1.164	1.5160 ²⁰			>112	
m431 m432	N-Methylthiourea N-Methyl-o-tolu- amide	CH ₃ NHC(=S)NH ₂ CH ₃ C ₆ H ₄ CONHCH ₃	90.15 149.19	4, 70 9, 465	1.16815		119–121 69–71			v s aq, alc
m433	N-Methyl-p-toluene- sulfonamide	CH ₃ C ₆ H ₄ SO ₂ NHCH ₃	185.25	11, 105			76–79			
m434	Methyl <i>p</i> -toluene-sulfonate	CH ₃ C ₆ H ₄ SO ₂ OCH ₃	186.23	11,99			27.5			
m435	Methyltriacetoxy- silane	CH ₃ Si(OOCCH ₃) ₃	220.3	4 ³ , 1896	1.175_4^{20}	1.40820		88 ^{3mm}		
m436	Methyl 2,2,2-tri- chloroacetimidate	Cl ₃ CC(=NH)OCH ₃	176.43	2, 212	1.425	1.4780 ²⁰		149	none	
m437	Methyltrichloro- germane	CH ₃ GeCl ₃	193.98		1.730			111		
m438	Methyl trifluoro- methanesulfonate	CF ₃ SO ₂ OCH ₃	164.10		1.450	1.3244 ²⁰		94–99	38	
m439	N-Methyl-N-tri- methylsilyl- acetamide	CH ₃ CON(CH ₃)- Si(CH ₃) ₃	145.3	4 ⁴ , 4011	1.439420	0.901 ²⁰		154		
m440	N-Methyl-N-(tri- methylsilyl)- trifluoroacetamide	CF ₃ CON(CH ₃)- Si(CH ₃) ₃	199.25		1.075	1.380220		132	25	
m441	Methyltripropoxy- silane	CH ₃ Si(OC ₃ H ₇) ₃	220.4		0.88_4^{20}	1.4085 ²⁰		83 ^{13mm}		
m442	(Methyl)triphenyl- phosphonium bromide	$[CH_3P(C_6H_5)_3]^+Br^-$	357.24				230–233			

m443	2-Methylundecanal	CH ₃ (CH ₂) ₈ CH(CH ₃)- CHO	184.32		0.830_4^{15}	1.432120		271	93	s alc, eth
m444 m445 m446 m447	Methyl urea Methyl vanillate Methyl vinyl ether 2-Methyl-5-vinyl-	CH ₃ NHCONH ₂ CH ₃ OC ₀ H ₃ (OH)COOCH ₃ CH ₃ OCH=CH ₂	74.08 182.18 58.08 119.17	4, 64 10, 396 1 ³ , 1857	1.204 0.7511 ²⁰ 0.898	1.3947 1.5437 ²⁰	101–102 64–65 –112	d 285–287 5.5 100 ^{50mm}	-56 65	v s aq, alc; i eth s hot alc, hot PE 0.8 aq; v s alc
m448	pyridine Morpholine		87.12	27, 5	1.007 ²⁰	1.4542 ²⁰	-4.9	128.9	35	misc aq, alc, bz, eth
m449	4-Morpholine- carbonitrile		112.12		1.109	1.4730^{20}		73 ^{0.6mm}	104	
m450	N-Morpholino-1- cyclohexene		167.25		0.995	1.5128^{20}		117–122	68	
m451	2-(N-Morpholino)- ethanesulfonic acid		195.24				>300			

4-Methyl-2-thiouracil, h120 Methyltrichlorosilane, t238 Methyltriethoxysilane, t266a Methyl trimethylacetate, m227 Methyltris(2-methoxyethoxy)silane, t429 β-Methylumbelliferone, h140 Methyluracil, d391 Methyl urethane, m181 Methyl valerate, m340 3-Methylvaleric acid, m342 4-Methylvaleronitrile, m339 Methyl veratrate, m225 Michler's ketone, b171 Monoethyl adipate, e149

Monoglyme, d439 Monomethyl adipate, m273 Monomethyl glutarate, m272 Monomethyl succinate, m274 Mordent violet 5, a60 4-Morpholinoethanol, h122 1-Morpholinocyclopentene, c361

1.31

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m452	3-(N-Morpholino)-		161.20		1.157		37–38	191 ^{30mm}	>112	
m453	1,2-propanediol β -Myrcene	(CH ₃) ₂ C=CHCH ₂ CH ₂ - C(=CH ₃)CH=CH ₃	136.24	1, 264	0.794_4^{20}	1.4709 ²⁰		166–168	39	s alc, chl, eth, HOAc
n1	1-Naphthaldehyde	C ₁₀ H ₇ CHO	156.18	7,400	1.150_4^{20}	1.6520^{20}	1–2	161 ^{15mm}	>112	s alc, eth
n2	Naphthalene	$C_{10}H_8$	128.17	5, 531	1.1624	1.5821100	80.2 subl above mp	217.7	78	0.3 aq; 7 alc; 33 bz; 50 chl
n3	1-Naphthalenecar- boxylic acid	C ₁₀ H ₇ COOH	172.18	9, 647			160–162	300		v s hot alc, eth
n4	1,5-Naphthalenedi- amine	$C_{10}H_6(NH_2)_2$	158.20	13, 203			185–187			s hot aq, hot alc
n5	1,8-Naphthalenedi- amine	$C_{10}H_6(NH_2)_2$	158.20	13, 204	1.1265499	1.682899	66.5	205 ^{12mm}		sl s aq; s alc, eth
n6	1-Naphthalene- methylamine	$C_{10}H_7CH_2NH_2$	157.22	12, 1316	1.073	1.6429 ²⁰		290–293	>112	
n7	1,8-Naphthalic anhydride		198.18	17, 521			267–269			sl s HOAc
n8	1,8-Naphthalimide		197.19	21, 527			300			sl s alc; i bz, eth,
n9	1-Naphthol	C ₁₀ H ₇ OH	144.17	6, 596	1.0954499	1.620699	96	288		v s alc, bz, chl, eth
n10	2-Naphthol	C ₁₀ H ₇ OH	144.17	6, 627	1.2174		121–123	285–286	161	0.1 aq; 125 alc; 6 chl; 77 eth; s alk
n11	1,4-Naphthoquinone		158.16	7,724	1.422		128	subl < 100		s bz, chl, eth, alk
n12	(2-Naphthoxy)acetic acid	C ₁₀ H ₇ OCH ₂ COOH	202.21	6, 645			155–157			
n13	2-(1-Naphthyl)- acetamide	C ₁₀ H ₇ CH ₂ CONH ₂	185.23	9,666			181–183			i aq; s bz, CS ₂

n14 n15	1-Naphthyl acetate 1-Naphthylacetic acid	C ₁₀ H ₇ OOCCH ₃ C ₁₀ H ₇ CH ₂ COOH	186.21 186.21	6, 608 9, 666			43–46 135	d		s alc, eth 3.3 alc; v s chl, eth
n16	1-Naphthylaceto- nitrile	$C_{10}H_7CH_2CN$	167.21	9, 667		1.6192^{20}	33–35	194 ^{18mm}	>112	s alc
n17	1-Naphthylamine	$C_{10}H_7NH_2$	143.18	12, 1212	1.123_{25}^{25}	1.6703	50	301	157	0.2 aq; v s alc, eth
n18	2-Naphthylsulfonic acid	$C_{10}H_7SO_3H$	208.23	11, 171	1.441 ²⁵		91	d		77 aq; s alc, eth
n19	1-(1-Naphthyl)-2- thiourea	$C_{10}H_7NHC(=S)NH_2$	202.28	12, 1241			198			0.6 aq; 2.4 acet; s alc
n20	Nicotine		162.24	23, 117	1.009740	1.5282 ²⁰	-79	123 ^{17mm}		misc aq; v s alc, eth, PE

MSTFA, m440

Mucic acid, t84

Mucochloric acid, d208

Myristolyl chloride, t41

Myristic acid, t39

Myristic acid, t40

Myristyl bromide b352

Naphthacene, b7

- 1-Naphthaleneacetamide, n13
- 1-Naphthaleneacetonitrile, n16

Naphthalenediols, d392, d393, d394, d395

1-Naphthol-2-carboxylic acid, h148 3-Naphthol-2-carboxylic acid, h149

1-Naphthol-3,6-disulfonic acid, h151

2-Naphthol-3,6-disulfonic acid, h150

1-Naphthonitrile, c293

(2-Naphthoxy)acetic acid, n12

N-1-Naphthylaniline, p130

Natural orange 6, h152

NBA, b218 NBS, b351

Neohexane, d489

Neohexene, d499

Neopentane, d592

Neopentyl alcohol, d595 Neopentyl glycol, d594

Neral, d563

Nerolidol, h184

Nicotinaldehyde, p256

Nicotinic acid, p256

Nicotinonitrile, c296

$$\begin{array}{c|c}
O & N-CH_2-H \\
N-CH_2-C-CH_2OH \\
OH
\end{array}$$

n20

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n21	Nitrilotriacetic	N(CH ₂ COOH) ₃	191.14	4, 369			246 d			0.1 aq; s hot alc
	acid									
n22	<i>m</i> -Nitroacetophenone	O ₂ NC ₆ H ₄ COCH ₃	165.15	7, 288			76–78	202		s alc, eth
n23	<i>p</i> -Nitroacetophenone	O ₂ NC ₆ H ₄ COCH ₃	165.15	7, 288			78–80	202		s alc
n24	o-Nitroaniline	O ₂ NC ₆ H ₄ NH ₂	138.13	12,687	1.44215		69–70	284		s hot aq, alc, chl
n25	<i>m</i> -Nitroaniline	O ₂ NC ₆ H ₄ NH ₂	138.13	12,698	1.43		114	306		0.1 aq; 5 alc; 6 eth
n26	<i>p</i> -Nitroaniline	O ₂ NC ₆ H ₄ NH ₂	138.13	12,711	1.43714		146	260 ^{100mm}	165	4 alc; 3.3 eth; s bz
n27	3-Nitrobenzaldehyde	O ₂ NC ₆ H ₄ CHO	151.12	7, 250	1.2792_4^{20}		58	164 ^{23mm}		s alc, chl, eth
n28	4-Nitrobenzaldehyde	O ₂ NC ₆ H ₄ CHO	151.12	7, 256	1.496		106-107			s alc, bz, HOAc
n29	2-Nitrobenzamide	O ₂ NC ₆ H ₄ CONH ₂	166.12	9, 373	1.462_4^{32}		174–178	317		s hot aq, hot alc,
										eth
n30	Nitrobenzene	C ₆ H ₅ NO ₂	123.11	5, 233	1.205_4^{15}	1.5546 ¹⁵	5.8	210.8	87	v s alc, bz, eth
n31	2-Nitrobenzene-1,4- dicarboxylic acid	O ₂ NC ₆ H ₃ (COOH) ₂	211.13	9, 851			270–272			
n32	3-Nitrobenzene-1,2-dicarboxylic acid	O ₂ NC ₆ H ₃ (COOH) ₂	211.13	9, 823			216 d			2 aq; v s hot alc
n33	4-Nitrobenzene-1,2-dicarboxylic acid	O ₂ NC ₆ H ₃ (COOH) ₂	211.13	9, 828			163–166			v s aq, alc; s eth
n34	5-Nitrobenzene-1,3-dicarboxylic acid	O ₂ NC ₆ H ₃ (COOH) ₂	211.13	9, 840			260–261			0.15 aq; v s alc, eth
n35	2-Nitrobenzene- sulfonyl chloride	O ₂ NC ₆ H ₄ SO ₂ Cl	221.62	11,67			65–67			s eth; d hot aq, alc
n36	6-Nitrobenzimidazole		163.14	23, 135			207-209			s alc, acid
n37	2-Nitrobenzoic acid	O ₂ NC ₆ H ₄ COOH	167.12	9,370	1.58		146–148			0.7 aq; 33 alc; 22 eth
n38	3-Nitrobenzoic acid	O ₂ NC ₆ H ₄ COOH	167.12	9, 376	1.494		142			0.3 aq; 33 alc; 40 acet
n39	4-Nitrobenzoic acid	O ₂ NC ₆ H ₄ COOH	167.12	9, 389	1.58		242.8			9 alc; 2 eth; 5 acet
	1	1	1	1	1	1	1	1	'	1

n40	4-Nitrobenzonitrile	O ₂ NC ₆ H ₄ CN	148.12	9,397	I		146–149	1		s HOAc; sl s aq,
		-20 4		.,						alc
n41	3-Nitrobenzoyl	O ₂ NC ₆ H ₄ COCl	185.57	9, 381			32–35	275–278		d aq, alc; v s eth
	chloride									
n42	4-Nitrobenzoyl chloride	O ₂ NC ₆ H ₄ COCl	185.57	9, 394			75	205 ^{105mm}		d aq, alc; s eth
n43	N-(p-Nitrobenzoyl)-	O ₂ NC ₆ H ₄ CONHCH ₂ COOH	224.17	9, 395			131-133			
	glycine									
n44	3-Nitrobenzyl	O ₂ NC ₆ H ₄ CH ₂ OH	153.14	6, 449			30–32	180 ^{3mm}		s aq, alc, eth
	alcohol									
n45	4-Nitrobenzyl	O ₂ NC ₆ H ₄ CH ₂ OH	153.14	6, 450			92–94	185 ^{12mm}		v s alc, eth; sl s aq
	alcohol									
n46	4-Nitrobenzyl	O ₂ NC ₆ H ₄ CH ₂ Br	216.04	5, 334			98–100			2 alc; v s eth
	bromide									
n47	4-Nitrobenzyl	O ₂ NC ₆ H ₄ CH ₂ Cl	171.58	5, 329			70–73			8 alc; s eth
	chloride				2.5	25				
n48	2-Nitrobiphenyl	$O_2NC_6H_4C_6H_5$	199.21	5, 582	1.44_4^{25}	1.613^{25}	36.7	325	179	s alc, acet, CCl ₄
n49	4-Nitrobiphenyl	$O_2NC_6H_4C_6H_5$	199.21	5, 583			112-114	340		sl s alc; v s eth
n50	1-Nitrobutane	CH ₃ CH ₂ CH ₂ CH ₂ NO ₂	103.18	1, 123	0.975_{20}^{20}	1.4112	-81.3	152.8		sl s aq; misc alc,
										eth
n51	3-Nitro-2-butanol	CH ₃ CH(NO ₂)CH(OH)CH ₃	119.12	1,373	1.1296_4^{25}	1.4414^{20}		92 ^{10mm}	91	
n52	2-Nitrodiphenylamine	O ₂ NC ₆ H ₄ NHC ₆ H ₅	214.22	12,690			76–78			i aq; s alc

Ninhydrin, i16 Nioxime, c323 2,2',2"-Nitrilotriethanol, t264 1,1',1"-Nitrilotris(2-propanol), t309

2-Nitro-*p*-anisidine, m79 5-Nitro-*o*-anisidine, m78 Nitroanisoles, m81, m82 4-Nitrobenzyl cyanide, n65 Nitrocresols, m323, m324

$$O_2N$$

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n53	Nitroethane	CH ₃ CH ₂ NO ₂	75.07	1,99	1.052820	1.3920 ²⁰	-90	114.1	30	4.5 aq; misc alc,
n54 n55	1-Nitroguanidine 5-Nitro-1 <i>H</i> -indazole	O_2 NNHC(=NH)NH ₂	104.07 163.14	3, 126 23, 129	25		d 225 207–209			eth; s alk, chl 0.4 aq; sl s MeOH s alc, bz, eth, acet
n56	Nitromethane	CH ₃ NO ₂	61.04	1,74	1.1322_4^{25}	1.3795^{25}	-28.4	101.2	35	11 aq; s alc, eth
n57	1-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	5, 553	1.223		59–60	304		s alc; v s chl, eth
n58	3-Nitro-2-pentanol	CH ₃ CH ₂ CH(NO ₂)- CH(OH)CH ₃	133.15	1, 385	1.0818425	1.4430 ²⁰		100 ^{10mm}	90	
n59	2-Nitrophenethyl alcohol	O ₂ NC ₆ H ₄ CH ₂ CH ₂ OH	167.16	6, 218	1.190	1.5637 ²⁰	2	267	>112	
n60	2-Nitrophenol	O2NC6H4OH	139.11	6, 213	1.495		44–45	214–216		s alc, bz, eth, alk
n61	4-Nitrophenol	O ₂ NC ₆ H ₄ OH	139.11	6, 226	1.495		112–114	279		s aq; v s alc, chl, eth
n62	4-Nitrophenyl acetate	O ₂ NC ₆ H ₄ OOCCH ₃	181.15	6, 233			77–79			s aq; v s alc, bz, eth
n63	2-Nitrophenylacetic acid	O ₂ NC ₆ H ₄ CH ₂ COOH	181.15	9, 454			139–142			s hot aq, alc
n64	4-Nitrophenylacetic	O ₂ NC ₆ H ₄ CH ₂ COOH	181.15	9, 455			153			s alc, bz, eth
n65	4-Nitrophenylaceto- nitrile	O ₂ NC ₆ H ₄ CH ₂ CN	162.15	9, 456			117			s alc, eth
n66	4-Nitrophenyl chloroformate	O ₂ NC ₆ H ₄ OOCCl	201.57	6 ¹ , 120			77–79	162 ^{19mm}		
n67	2-Nitro- <i>p</i> -phenylene-	$O_2NC_6H_3(NH_2)_2$	153.14	13, 120			137–140			
n68	4-Nitro- <i>o</i> -phenylene-	$O_2NC_6H_3(NH_2)_2$	153.14	13, 29			199–201			s acid
n69	4-Nitrophenyl- hydrazine	O ₂ NC ₆ H ₄ NHNH ₂	153.14	15, 468			156 d			s alc, chl, eth, hot bz

n70	2-Nitrophenyl phenyl ether	O ₂ NC ₆ H ₄ OC ₆ H ₅	215.21	$6^2,222$	1.2539 ²²	1.575^{20}	<-20	184 ^{8mm}		s alc, eth
n71	4-Nitrophenyl phenyl ether	O ₂ NC ₆ H ₄ OC ₆ H ₅	215.21	6, 232			53–56	320		s bz, eth
n72	3-Nitrophthalic anhydride		193.11	17, 486			163–165			sl s aq, bz
n73	1-Nitropropane	CH ₃ CH ₂ CH ₂ NO ₂	89.09	1, 115	1.0009 ²⁰	1.4016^{20}	-104.0	131.2	33	1.4 aq; misc alc, eth
n74	2-Nitropropane	(CH ₃) ₂ CHNO ₂	89.09	1,116	0.9876^{20}	1.3949 ²⁰	-91.3	120.3	37	1.7 aq; misc alc, eth
n75	2-Nitro-1-propanol	CH ₃ CH(NO ₂)CH ₂ OH	105.09	1,358	1.1841_4^{25}	1.4379^{20}		99 ^{10mm}	100	s aq, alc, eth
n76	4-Nitropyridine- N-oxide	$O_2NC_5H_4N(O)$	140.10				159–162			_
n77	8-Nitroquinoline		174.16	20, 373			89-91			s alc, bz, eth; i aq
n78	Nitrosobenzene	C ₆ H ₅ NO	107.11	5, 230			67–69	59 ^{18mm}		i aq; s alc
n79	N-Nitrosodi- methylamine	(CH ₃) ₂ NNO	74.08	8, 84	1.0048420	1.4368 ²⁰		151–153	61	v s aq, alc, eth
n80	<i>p</i> -Nitrosodi- phenylamine	C ₆ H ₅ NHC ₆ H ₄ NO	198.22				144–145			v s alc, bz, chl, eth
n81	1-Nitroso-2-naphthol	$C_{10}H_6(NO)OH$	173.16	7,712			109–110			3 alc; s bz, eth, alk

Nitroglycerin, g21

5-Nitroisophthalic acid, n34

3-Nitrophenyl disulfide, b194

4-Nitrophenyl disulfide, b195

4-(p-Nitrophenylthio)aniline, a243

3-Nitro-*o*-phthalic acid, n32

4-Nitro-o-phthalic acid, n33

N-Nitrosophenylhydroxylamine, c284

$$O_2N$$
 N
 N
 H

n55

n77

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n82	1-Nitroso-2- naphthol-3,6-di- sulfonic acid, di-Na salt hydrate		377.26	11², 190			>300			2.5 aq; sl s alc
n83	4-Nitrosophenol	ONC ₆ H ₄ OH	123.11	7,622			d 126			s aq; v s alc, eth; explodes on contact with conc acid, alk, or fire
n84	β -Nitrostyrene	C ₆ H ₅ CH=CHNO ₂	149.15	5, 478			58	250		s alc; v s eth
n85	2-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 318	1.1622_{15}^{19}	1.547220	-10	222	106	s alc, bz
n86	3-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 321	1.1581_4^{20}	1.5459^{20}	15.5	231.9	101	misc alc, eth; s bz
n87	4-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 323	1.392		53-54	238	106	s alc, bz, chl, eth
n88	2-Nitro-α,α,α- trifluorotoluene	CF ₃ C ₆ H ₄ NO ₂	191.11	$5^2, 251$			31–32	105 ^{20mm}		v s alc, bz
n89	3-Nitro-α,α,α- trifluorotoluene	CF ₃ C ₆ H ₄ NO ₂	191.11	5, 327	1.43646	1.4715 ²⁰	-2.4	200–205	87	s alc, eth
n90	Nonadecane	CH ₃ (CH ₂) ₁₇ CH ₃	268.51	1, 174	0.7776_4^{32}	1.433538	31.9	330.6	168	s eth; sl s alc
n91	1,8-Nonadiyne	HC≡C(CH ₂) ₅ C≡CH	120.20	$1^2, 248$	$0.8159_4^{\frac{7}{21}}$	1.4492^{20}	-21	55 ^{13mm}	41	·
n92	Nonane	CH ₃ (CH ₂) ₇ CH ₃	128.26	1, 165	0.7176_4^{20}	1.4054^{20}	-53.5	150.8	31	s abs alc, eth
n93	1,9-Nonanediamine	$H_2N(CH_2)_9NH_2$	158.29	4, 272			37–38	258		
n94	Nonanedinitrile	NC(CH ₂) ₇ CN	150.23	2,709	0.929	1.4460^{20}		176 ^{11mm}	>112	v s alc, bz, eth
n95	1,9-Nonanedioic acid	HOOC(CH ₂) ₇ COOH	188.22	2,707	1.029_4^{20}		106.5	286 ^{100mm}		0.24 aq; v s alc; 3 eth
n96	1,9-Nonanediol	HO(CH ₂) ₉ OH	160.26	1,493			45-47	177 ^{15mm}		
n97	Nonanenitrile	CH ₃ (CH ₂) ₇ CN	139.24	2,354	0.821_4^{15}	1.426020	-34.2	224.0	81	s alc, eth
n98	Nonanoic acid	CH ₃ (CH ₂) ₇ COOH	158.24	2,352	0.906_4^{20}	1.433020	12.5	254	100	s alc, chl, eth
n99	1-Nonanol	CH ₃ (CH ₂) ₈ OH	144.26	1, 423	0.8274_4^{20}	1.4338 ²⁰	-5.5	213.1	75	0.6 aq; misc alc, eth
n100	5-Nonanone	$(C_4H_9)_2CO$	142.24	1,710	0.806_4^{20}	1.4190^{20}	-50	187	60	misc alc, eth

n101 Nonanoy	l chloride	CH ₃ (CH ₂) ₇ COCl	176.69	2, 353	0.946_4^{15}	1.4377 ²⁰	-60.5	215.4	81	d aq, alc: s eth
n102 1-Nonen	e 1	$H(CH_2)_7CH = CH_2$	126.24	$1^2, 202$	0.7292^{20}	1.4157^{20}	-81.4	146.9	46	_
n103 Nonyl ald	lehyde	CH ₃ (CH ₂) ₇ CHO	142.24	1,708	0.827_{19}^{19}	1.4240^{20}		185	63	
n104 Nonylam	ine	CH ₃ (CH ₂) ₈ NH ₂	143.27	4, 198	0.782	1.4330^{20}		201	62	sl s aq; s alc, eth
n105 Nopol			166.26		0.973	1.4930^{20}		230-240	98	_
n106 Nopyl ac	etate		210.3		0.9805^{25}	1.4721^{20}				
n107 Norborna	ine		96.17	$5^2, 45$			82-84			s alc
n108 2-Norbor	nanone		110.16	7,57			88-91	168-172	33	
n109 trans-5-N	Iorbornene-		219.07		1.349	1.5165^{20}		118 ^{11mm}	110	
2,3-dic	arbonyl									
dichlo	ride									

Nitroso-R-salt, n82 Nitroterephthalic acid, n31 2-Nitro-*p*-toluidine, m317 4-Nitro-*o*-toluidine, m315 5-Nitro-*o*-toluidine, m316 4-Nitroveratrole, d444 Nitroxylenes, d556, d557, d558, d559 Nonyl alcohol, n99 2,5-Norbornadiene, b129 exo-2-Norbornanamine, a250 5-Norbornen-2-carbaldehyde, b131 Norbornene, b130

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n110	5-Norbornen-2-yl		152.19		1.044	1.470020		76 ^{14mm}	62	
	acetate		140.10		1.040	1.462220		67 ^{16mm}		
n111	exo-2-Norbornyl formate		140.18		1.048	1.4622 ²⁰		6/1011111	53	
n112	(+)-Norephedrine		187.67	13 ² , 371			174–176			
	HC1									
o1	(Z,Z)-9,12-Octa-	CH ₃ (CH ₂) ₄ CH=CHCH ₂ -	280.44	2, 496	0.9025_4^{20}	1.4699^{20}	-5	230 ^{16mm}		v s eth; misc PE;
	decadienoic acid	$CH = CH(CH_2)_7COOH$	202.50				100 100	0.54.12mm		s abs alc
o2	Octadecanamide	CH ₃ (CH ₂) ₁₆ CONH ₂	283.50	2, 384	28	20	108–109	251 ^{12mm}		s hot alc, hot eth
03	Octadecane	$CH_3(CH_2)_{16}CH_3$	254.50	1, 173	0.7767_4^{28}	1.4367 ²⁸	28.2	316.7	165	s acet, eth; sl s alc
04	1-Octadecanethiol	$CH_3(CH_2)_{17}SH$	286.57			1.4648	29–31	360	185	s eth; sl s alc
05	Octadecanoic acid	CH ₃ (CH ₂) ₁₆ COOH	284.48	2, 377	0.847 ⁷⁰	1.429980	70	383		4.9 alc; 20 bz; 50
- (1-Octadecanol	CH (CH) OH	270.50	1 421	0.812358	1.438820	57.9	203 ^{10mm}		chl; 3.9 acet
06		CH ₃ (CH ₂) ₁₇ OH	270.50	1,431			37.9		> 110	s alc, eth
о7	9,12,15-Octadeca- trienoic acid	CH ₃ (CH ₂ CH=CH) ₃ CH ₂ - (CH ₂) ₆ COOH	278.44	2, 499	0.791_4^{18}	1.4800^{20}		230 ^{17mm}	>112	s alc, bz, eth
08	1-Octadecene	$CH_3(CH_2)_1CH=CH_2$	252.49	1, 226	0.791^{18}_{4}	1.443920	17.7	314.9	148	s hot acet
08	9-Octadecen-1-amine	3 2/13 2	267.50	1,220	0.7914	1.4439	17.7	314.9	154	s not acet
09	9-Octadecen-1-amine	$CH_3(CH_2)_7CH = CH - (CH_2)_8NH_2$	267.50		0.813	1.45/829			154	
o10	(Z)-9-Octadecenoic	CH ₃ (CH ₂) ₇ CH=CH-	282.47	2, 463	0.8906_4^{20}	1.457120	4	286 ^{100mm}		misc alc, eth; s bz,
	acid	(CH ₂) ₇ COOH								chl
o11	(E)-9-Octadecenoic	CH ₃ (CH ₂) ₇ CH=CH-	282.47	$2^2,441$	0.85179	1.430899	44–45	288 ^{100mm}		s bz, chl, eth
	acid	(CH ₂) ₇ COOH								
o12	(Z)-9-Octadecen-	CH ₃ (CH ₂) ₇ CH=CH-	268.49	1, 453	0.849_4^{20}	1.4610^{20}	13-19	195 ^{8mm}	>112	s alc, eth
	1-01	(CH ₂) ₈ OH								
o13	Octadecylamine	CH ₃ (CH ₂) ₁₇ NH ₂	269.52	4, 196	0.777^{27}		50-52	232 ^{32mm}	148	s alc, bz, eth
o14	Octadecyl	CH ₃ (CH ₂) ₁₇ NCO	295.51		0.847	1.4501^{20}		170 ^{2mm}	185	
	isocyanate									
	1	'		'		'	'	'		1

o15	Octadecyltri- chlorosilane	CH ₃ (CH ₂) ₁₇ SiCl ₃	387.94		0.984	1.4602^{20}		223 ^{10mm}	89	
o16	Octadecyl vinyl ether	$CH_3(CH_2)_{17}OCH = CH_2$	296.54		0.821430	1.4440 ³⁰	28	187 ^{5mm}	177	
o17	1,7-Octadiene	$H_2C = CH(CH_2)_4CH = CH_2$	110.20		0.746	1.422120		114–121	9	
o18	1 <i>H</i> ,1 <i>H</i> ,5 <i>H</i> -Octa-	HCF,CF,CF,CH,OH	232.08		1.664720	1.3190^{20}		140-141	74	
	fluoro-1-pentanol									
o19	Octamethylcyclo-	[—(CH ₃) ₂ SiNH—] ₄	292.7		0.95^{22}	1.458^{25}		224-225		
	tetrasilazane									
o20	Octamethylcyclo-	[—(CH ₃) ₂ SiO—] ₄	296.62		0.9558^{20}	1.3968^{20}	17.5	175	90	
	tetrasiloxane									
o21	Octamethyltri-	[(CH ₃) ₃ SiO] ₂ -	236.0		0.8200^{20}	1.3848^{20}	~-80	152-153	38	s bz, PE; sl s alc
	siloxane	Si(CH ₃) ₂								
o22	Octane	CH ₃ (CH ₂) ₆ CH ₃	114.23	1, 159	0.7025_4^{20}	1.3974^{20}	-56.8	125.7	15	s eth; sl s alc
o23	1,8-Octanediamine	$H_2N(CH_2)_8NH_2$	144.26	4, 271			50-52	225	165	
o24	1,8-Octanedioic	HOOC(CH ₂) ₆ COOH	174.20	2, 691			140-144	230 ^{15mm}		0.16 aq; 0.6 eth; s
	acid									alc
o25	1,2-Octanediol	CH ₃ (CH ₂) ₅ CH(OH)-	146.23	$1^3, 2217$			36–38	132 ^{10mm}	>112	
		CH ₂ OH								

Norbornylene, b130 Norcamphor, n107 Norleucine, a183 Norvaline, a253 NTA, n21 Octadecyl bromide, b319 Oxtadecyl mercaptan, o4 2,3,4,6,7,8,9,10-Octahydropyrimido [1,2-a]azepine, d46 Octaldehyde, o40 Octamethylene glycol, o26 Octanal, o40 1,8-Octanedicarboxylic acid, d9

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
o26	1,8-Octanediol	HO(CH ₂) ₈ OH	146.23	1,490			59–61	172 ^{20mm}		v s alc; sl s aq, eth
o27	Octanenitrile	CH ₃ (CH ₂) ₆ CN	125.22	2, 349	0.8135^{20}	1.4202^{20}	-45.6	205.2	73	s eth; sl s alc
o28	1-Octanethiol	CH ₃ (CH ₂) ₇ SH	146.30	1 ³ , 1710	0.843	1.452520	-49.2	199.0	68	s alc
o29	Octanoic acid	CH ₃ (CH ₂) ₆ COOH	144.21	2, 347	0.9088_4^{20}	1.427920	16.6	239.3	110	0.07 aq; v s alc,
		3. 20								chl, eth, PE
o30	1-Octanol	CH ₃ (CH ₂) ₇ OH	130.23	1,418	0.8258_4^{20}	1.4296^{20}	-15.0	195.2	81	0.06 aq; misc alc,
										chl, eth
o31	DL-2-Octanol	CH ₃ (CH ₂) ₅ CH(OH)CH ₃	130.23	1,419	0.8207_4^{20}	1.4202^{20}	-38.6	179-180	71	0.08 aq; misc alc,
										eth
o32	DL-3-Octanol	CH ₃ (CH ₂) ₄ CH(OH)-	130.23	1 ¹ , 208	0.8216^{20}	1.426220		174–176	65	
		CH ₂ CH ₃								
o33	4-Octanol	CH ₃ (CH ₂) ₃ CH(OH)-	130.23		0.8192^{20}	1.425^{20}		176.6	71	
		CH ₂ CH ₂ CH ₃								
o34	2-Octanone	CH ₃ (CH ₂) ₅ COCH ₃	128.22	1,704	0.819_4^{20}	1.4150^{20}	-16	173	62	i aq; misc alc, eth
o35	3-Octanone	CH ₃ (CH ₂) ₄ COCH ₂ CH ₃	128.22	1,706	0.8220_4^{20}	1.4150^{20}		167–168	46	i aq; misc alc, eth
o36	4-Octanone	CH ₃ (CH ₂) ₃ COCH ₂ -	128.22	1,706	0.809	1.4139^{20}		164	45	
		CH ₂ CH ₃								
o37	Octanoyl chloride	CH ₃ (CH ₂) ₆ COCl	162.66	2, 348	0.955_{15}^{15}	1.4350^{20}	< -70	195	75	d aq, alc; s eth
o38	Octaphenylcyclo-	$[-(C_6H_5)_2SiO-]_4$	793.2		1.185			340 ^{1mm}		s alc, bz, HOAc
	tetrasiloxane									
o39	1-Octene	$CH_3(CH_2)_5CH = CH_2$	112.22	1, 221	0.7149_4^{20}	1.408720	-101.7	121.3	21	i aq; misc alc, eth
o40	Octyl aldehyde	CH ₃ (CH ₂) ₆ CHO	128.22	1,704	0.821_4^{20}	1.418320	12–15	163.4	51	sl s aq; misc alc
o41	Octylamine	$CH_3(CH_2)_7NH_2$	129.25	4, 196	0.782	1.4290^{20}	-5 to	175–177	62	i aq; s alc, eth
							-1	4.0		
o42	4-Octylaniline	$CH_3(CH_2)_7C_6H_4NH_2$	205.35	12, 1185	20	20		175 ^{13mm}		
o43	Octyltrichlorosilane	CH ₃ (CH ₂) ₇ SiCl ₃	247.7		1.0720	1.447 ²⁰		226 ^{730mm}		
o44	1-Octyne	$CH_3(CH_2)_5C \equiv CH$	110.19	1, 258	0.7457^{20}	1.4159^{20}	-79.3	126.2		i aq; s alc, eth
o45	1-Octyn-3-ol	CH ₃ (CH ₂) ₄ CH(OH)-	126.20		0.864	1.4410^{20}			63	
		C≡CH								

o46	L-(+)-Ornithine	H ₂ N(CH ₂) ₃ CH(NH ₂)- COOH	132.16	4,420			142			v s aq, alc; sl s eth
o47	Oxacycloheptane	Coon	100.16		0.890	1.440^{20}		122	10	
o48	Oxalic acid	НООССООН	90.04	2,502	1.90^{17}_{4}		189 d			9.5 aq; 24 alc; 1.3
										eth
o49	Oxalic acid	HOOCCOOH-2H ₂ O	126.07	2,502	1.65349		$-2H_2O$,			14 aq; 40 alc; 1 eth
	dihydrate						102			
o50	Oxalyl bromide	BrCO—COBr	215.84			1.5220		103 ^{720mm}	none	
o51	Oxalyl chloride	CICO—COCI	126.93	2,542	1.488_4^{13}	1.4340^{13}	-12	64	none	s eth; violent d aq,
										alc
o52	Oxalyl dihydrazide	H ₂ NNHCO—CONHNH ₂	118.10	2, 559			240 d			s hot aq; sl s alc,
										eth
o53	Oxamic hydrazide	H ₂ NCO—CONHNH ₂	103.08	2,559			218 d			s alk; sl s aq; i eth
o54	Oxamide	H ₂ NCO—CONH ₂	88.07	2, 545	1.667_4^{20}		d 350			sl s hot aq, alc
o55	2-Oxazolidone		87.08	27, 135			86–89	220 ^{48mm}		
o56	2-Oxobutyric acid	$CH_3CH_2C(=O)COOH$	102.09	3, 629	1.200_4^{17}	1.3972^{20}	32-34	82 ^{16mm}		v s aq, alc; v sl s
	1	1	ı	1	1	I	1	1	I	eth

tert-Octylamine, t102 Octyl bromide, b320 Octyl cyanide, n97 Octyl chloride, c190 Octyl iodide, i46 Oleic acid, o11 Oleyl alcohol, o12 Oleylamine, o9 Orthanolic acid, a118
7-Oxabicyclo[2.2.1]heptane, e6
7-Oxabicyclo[4.1.0]heptane, e5
6-Oxabicyclo[3.1.0]hexane, e9
2-Oxabicyclo[6.1.0]nonane, e7a
Oxacyclobutane, t345
Oxacyclopentane, t66
Oxalylurea, i6

1,4-Oxathiane, t164
Oxepane, o47
Oxetane, t345
Oxirane, e129
2-Oxo-10-bornanesulfonic acid, c7
3-Oxobutanoic acid, a24
3-Oxobutyraldehyde dimethyl acetal, d435

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
057	2-Oxohexamethyl- eneimine		113.16	21 ² , 216	1.02 ⁷⁵	1.4935	69.2	180 ^{50mm}		84 aq
o58 o59	4-Oxopentanoic acid 2-Oxopropional- dehyde	CH ₃ COCH ₂ CH ₂ COOH CH ₃ COCHO	116.12 72.06	3, 671 1, 762	$ \begin{array}{c c} 1.1447_4^{25} \\ 1.0455^{24} \end{array} $	1.4396 ²⁰ 1.4209 ²⁰	33–35	245.8 72	137 none	v s aq, alc, bz, eth s aq, alc
o60 o61	2-Oxopropionic acid 2,2'-Oxydiacetic acid	CH ₃ COCOOH HOOCCH ₂ OCH ₂ COOH	88.06 134.09	3, 608 3, 234	1.267 ₄ ¹⁵	1.4315 ²⁰	11.8 142–145	165 d d	82	misc aq, alc, eth v s aq, alc; sl s eth
o62 o63	4,4'-Oxydianiline 3,3'-Oxydipropio- nitrile	H ₂ NC ₆ H ₄ OC ₆ H ₄ NH ₂ NCCH ₂ CH ₂ OCH ₂ CH ₂ CN	200.24 124.14	13, 441	1.043	1.4405 ²⁰	190 d	112 ^{0.5mm}	>112	
p1	Paraformaldehyde	(CH ₂ O) _x		1,566			156 d		71	slowly s aq; s alk; i alc, eth
p2 p3	Paraldehyde Parathion	$[-CH(CH_3)O-]_3$ $(C_2H_5O)_2P(=S)(O)-$ $C_6H_4NO_7$	132.16 291.27	19, 385	$0.9984^{15} \\ 1.26_4^{25}$	1.4049 ²⁰ 1.5370 ²⁵	12.5 6	124 375		11 aq; misc alc, chl v s alc, bz, eth
p4 p5	DL-Patchenol Pentabromoethyl- benzene	CH ₃ CH ₂ C ₆ Br ₅	166.26 500.67	6 ² , 64 5, 357	0.987	1.5045 ²⁰	137–139	234–238	107	
p6 p7 p8	Pentabromophenol Pentachloroacetone Pentachlorobenzene	C ₆ Br ₅ OH Cl ₂ CHCOCCl ₃ C ₆ HCl ₅	488.62 230.31 250.34	6, 206 1, 656 5, 205	1.690 1.8342 ¹⁶	1.4967 ²⁰	223–226 21 anhyd 82–85	subl 192 275–277	none	sl s alc, eth i aq; v s acet v s bz, chl, eth
p9	Pentachloroethane	Cl ₂ CHCCl ₃	202.30	1,87	1.6712_4^{25}	1.5030^{20}	-29.0	160.5	none	0.05 aq; misc alc, eth
p10	Pentachloronitro- benzene	C ₆ Cl ₅ NO ₂	295.34	5, 247	1.718_4^{25}		140–143			s bz, chl
p11	Pentachlorophenol	C₀Cl₅OH	266.34	6, 194	1.978422		190–191	310 d		v s alc; s bz; 148 eth
p12	Pentachloropyridine	C ₅ Cl ₅ N	251.33	20, 232			124–126			

p13 p14 p15	Pentadecane 8-Pentadecanone 3-Pentadecylphenol	CH ₃ (CH ₂) ₁₃ CH ₃ [CH ₃ (CH ₂) ₆] ₂ CO C ₁₅ H ₃₁ C ₆ H ₄ OH	212.42 226.40 304.52	1, 172 1, 717	0.7684 ₄ ²⁰	1.4319 ²⁰	9.9 41–43 45–48	270.6 178 195 ^{1mm}	132	v s alc, eth s alc
p16	1,2-Pentadiene	CH ₃ CH ₂ CH=C=CH ₂	68.12	1, 251	0.6926_4^{20}	1.420920	-137.3	44.9	20	
p17 p18	(<i>E</i>)-1,3-Pentadiene (<i>Z</i>)-1,3-Pentadiene	CH ₃ CH=CHCH=CH ₂ CH ₂ CH=CHCH=CH ₃	68.12 68.12	1, 251 1, 251	$0.6760^{20} \ 0.6910^{20}$	1.4301^{20} 1.4363^{20}	-87.5 -140.8	42.0 44.1	$-28 \\ -28$	
p19	1,4-Pentadiene	H ₂ C=CHCH ₂ CH=CH ₂	68.12	1, 251	0.6608_4^{22}	1.3888^{20}	-148.3	26.0	4	
p20	Pentaerythritol	C(CH ₂ OH) ₄	136.15	1,528	1.38425	1.548	260	subl		6 aq; v sl s alc; i eth
p21	Pentaerythrityl tetrabromide	C(CH ₂ Br) ₄	387.76	1, 142			158–160	305–306		
p22	Pentaerythrityl tetranitrate	C(CH ₂ ONO ₂) ₄	316.15	1², 602	1.77340		140		sensi- tive to shock; ex- plodes on percu- ssion	acet; sl s eth, alc

3-Oxo-N-phenylbutanamide, a32

2,2'-Oxybis(chloroethane), b158

1,1'-Oxybis(2-methylpropane), d407

1,1'-Oxybis(pentane), d651

3,3'-Oxybis(1-propene), d26

2,2'-Oxydiethanethiol, b186

2,2'-Oxydiethanol, b181 Palmitic acid, h35 Pamoic acid, m235 Parabanic acid, i6 Pelargonaldehyde, n103 Pelargonic acid, n98

Pelargonoyl chloride, n101 Pelargononitrile, n97 Pentabromophenyl ether, b197 Pentaerythritol diformal, t126

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

1,2,3,4,5-Pentamethylcyclopentadiene 1,5-Pentamethylcyclopentadiene 138.17 26², 213 1,976 1,9412mm 12 12 1,000 1,5-Pentamethylcyclopentadiene 138.17 26², 213 1,076 0.8095¼0 1.3942²0 -92 102-103 12 12 1,5-Pentamediamine H₂N(CH₂CH₂CH₃ 1,5-Pentamediamine H₂N(CH₂)NH₂ 102.18 4,266 0.873¼5 1.4591²0 -129.7 178-180 62 1,5-Pentamedione Ho(CH₂)NH₂ 102.18 4,266 0.873¼5 1.4591²0 -129.7 178-180 62 1,5-Pentamedione CH₃CH₂COCOCH₃ 100.11 1,776 0.957 1.4068²0 -52 110-112 19 19 1,776 1	h Solubility in 100 parts solvent
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
1,2,3,4,5-Pentamethylcyclopentadiene 136.24 136.24 136.24 1373 ²⁰ 1,4733 ²⁰ 1,4404 ²⁰ 1,4494 ²⁰ 1,4494 ²⁰ 1,494 ²⁰	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	v s alc, bz
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.4 aq; misc alc, eth
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	misc alc, eth
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	s aq, alc; sl s eth
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	s aq, alc; sl s eth
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	17 aq; misc alc, eth
acid, Na salt 1-Pentanethiol Pentanoic acid 1-Pentanol CH ₃ (CH ₂) ₄ SH CH ₃ (COOH 102.13 1-Pentanol CH ₃ (CH ₂) ₄ OH 104.22 1, 384 0.840 0.840 0.9390 ²⁰ 0.9390 ²⁰ 1.4460 ²⁰ 0.9390 ²⁰ 1.4080 ²⁰ 0.9390 ²⁰ 1.4100 ²⁰ 0.8148	i aq; s alc, eth
p36 Pentanoic acid CH ₃ (CH ₂) ₃ COOH 102.13 2,299 0.9390 ₄ ²⁰ 1.4080 ²⁰ -33.7 185.5 88 1-Pentanol CH ₃ (CH ₂) ₄ OH 88.15 1,383 0.8148 ₄ ²⁰ 1.4100 ²⁰ -78.9 137.8 32	4 aq
p37 1-Pentanol $CH_3(CH_2)_4OH$ 88.15 1,383 0.8148_4^{20} 1.4100^{20} -78.9 137.8 32	i aq; misc alc, eth
	2.4 aq; v s alc, eth
2.9 2. Domestanol CII CII CII CII CII CII CII CII CII CI	2.7 aq; misc alc, eth
p38 2-Pentanol $CH_3CH_2CH_2CH(OH)CH_3$ 88.15 1,384 0.8393 $_4^{20}$ 1.4064 $_2^{20}$ glass 119.0 40	16.6 aq; misc alc, eth
p39 3-Pentanol CH ₃ CH ₂ CH ₁ OH)CH ₃ CH ₃ 88.15 1,385 0.8150 ₄ ²⁵ 1.4079 ²⁵ -69 115.6 40	5.2 aq; s alc, eth
p40 γ-Pentanolactone 100.12 17, 235 1.057 1.4330 -31 207-208 81	_
p40a δ -Pentanolactone 100.12 17, 235 1.079 1.4575 ²⁰ 60 ^{0.5mm} 100	

p41	2-Pentanone	CH ₃ CH ₂ CH ₂ COCH ₃	86.13	1,676	0.8095^{20}	1.3903	-77.8	101.7	7	misc acet, bz, eth, PE
p42	3-Pentanone	CH ₃ CH ₂ COCH ₂ CH ₃	86.13	1,679	0.8143^{20}	1.3923^{20}	-39.0	102.0	12	3.4 aq
p43	Pentanophenone	C ₆ H ₅ CO(CH ₂) ₃ CH ₃	162.23	7, 327	0.988	1.5143^{20}		107 ^{5mm}	102	s alc, eth
p44	Pentanoyl chloride	CH ₃ CH ₂ CH ₂ COCl	120.58	2, 301	1.016	1.4216^{20}		125-127	23	
p45	1,4,7,10,13-Penta-	[—CH ₂ CH ₂ O—] ₅	220.27			1.4615^{20}		135 ^{0.2mm}		
	oxacyclo-									
	pentadecane									
p46	3,6,9,12,15-Penta-	CH ₃ O(CH ₂ CH ₂ O) ₄ CH ₂ -	252.31		0.933	1.4500^{20}		133 ^{0.005mm}	>112	
	oxahexadecanol	CH₂OH								
p47	1-Pentene	$CH_3CH_2CH=CH_2$	70.14	1,210	0.6410_4^{20}	1.3714^{20}	-165.2	30.0		misc alc, bz, eth
p48	(E)-2-Pentene	CH ₃ CH ₂ CH=CHCH ₃	70.14	1,210	0.6482_4^{20}	1.3793^{20}	-140.2	36.3	-45	misc alc, eth
p49	(Z)-2-Pentene	CH ₃ CH ₂ CH=CHCH ₃	70.14	1,210	0.6503_4^{20}	1.3830^{20}	-151.4	36.9		misc alc, eth
p50	4-Pentenoic acid	H ₂ C=CHCH ₂ CH ₂ COOH	100.11	2, 425	0.9843_4^{18}	1.4341^{18}	<-18	187-189		sl s aq; s alc, eth
p51	3-Penten-2-one	CH ₃ CH=CHCOCH ₃	84.12	1,732	0.8624_4^{20}	1.4405^{20}		121-124	21	s aq
p52	Pentyl acetate	CH ₃ (CH ₂) ₄ OOCCH ₃	130.19	2, 131	0.8753^{20}	1.4028^{20}	<-100	149.2	23	0.17 aq
p53	Pentylamine	CH ₃ (CH ₂) ₄ NH ₂	87.17	4, 175	0.752	1.4110^{20}	-55	104	4	v s aq; misc alc,
										eth
p54	Pentylbenzene	$CH_3(CH_2)_4C_6H_5$	148.25	5, 434	0.8594_4^{20}	1.4885^{20}	-78.3	202.2	65	s alc; misc bz, eth
•	1 *									

Pentalin, p9 pentamethylene glycol, p30 Pentamethylene oxide, t76 Pentamethylethyl alcohol, t338 1,5-Pentanedicarboxylic acid, h8 Pentanedinitrile, g14 Pentanedioic acid, g11 2,5,8,11,14-Pentaoxapentadecane, b190

Penetetic acid, d299 sec-Pentylamine, a251 tert-Pentylamine, d601

$$CH_3$$
 CH_3 CH_3

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p55	4- <i>tert</i> -Pentylcyclo-hexanone		168.28	73, 173	0.920	1.4677 ²⁰		125 ^{16mm}	104	
p56	4- <i>tert</i> -Pentylphenol	CH ₃ CH ₂ C(CH ₃) ₂ - C ₆ H ₄ OH	164.25	6, 548	0.962420		93	262.2		s alc, eth
p57 p58	1-Pentyne L-Perillaldehyde	CH ₃ CH ₂ CH ₂ C≡CH	68.11 150.22	1, 250 7, 158	$0.6901_4^{20} \\ 0.9645_4^{20}$	$1.3852^{20} 1.5072^{20}$	-105.7	40.2 105 ^{10mm}	95	v s alc; misc eth
p59	Peroxyacetic acid	CH ₃ C(=0)OOH	76.05		1.22645		0.1	105 explodes 110		v s aq, alc, eth
p60	Petroleum ether	principally pentanes and hexanes			0.640			35–80	-40	misc bz, chl, eth, CCl ₄
p61	Phenanthrene		178.23	5, 667	1.179 ²⁵		100	340		1.6 alc; 50 bz; 30 eth
p62	9,10-Phenanthrene- dione		208.22	7, 796	1.4054		209–211			s bz, eth, hot alc
p63	1,10-Phenanthroline		180.21	23, 227			117			1.4 bz; s alc, acet
p64	Phenol	C ₆ H ₅ OH	94.11	6, 110	1.0576_4^{41}	1.541841	40.9	181.8	79	6.7 aq; 8.2 bz; v s alc, chl, eth, alk
p65	Phenolphthalein		318.33	18, 143	1.299425		258–262			8.2 alc; 1 eth
p66	Phenothiazine		199.28	27, 63			185.1	371		v s bz; s eth; sl s alc
p67	Phenothiazine-10- carbonyl chloride		261.73	27, 66			168–171			
p68	Phenoxyacetic acid	C ₆ H ₅ OCH ₂ COOH	152.15	6, 161			98	285 sl d		1.3 aq; v s alc, bz, HOAc, CS ₂ , eth
p69	Phenoxyacetyl chloride	C ₆ H ₅ OCH ₂ COCl	170.60	6, 162	1.235	1.5340^{20}		225–256		d aq, alc; s eth
p70	<i>p</i> -Phenoxyaniline	C ₆ H ₅ OC ₆ H ₄ NH ₂	185.23	13, 438			82–84	189 ^{14mm}		s hot aq; v s alc, eth

p71	2-Phenoxybutyric	CH ₃ CH ₂ CH(OC ₆ H ₅)-	180.20	6, 163			79–83	258		sl s aq
	acid	COOH								
p72	2-Phenoxyethanol	C ₆ H ₅ OCH ₂ CH ₂ OH	138.17	6, 146	1.102_4^{22}	1.5370^{20}	14	245.2	110	s aq; v s alc, eth
p73	1-Phenoxy-2-propanol	C ₆ H ₅ OCH ₂ CH(OH)CH ₃	152.19	$6^1, 85$	1.06325	1.523^{20}	13-18	240	135	
p74	Phenoxy-2-propanone	C ₆ H ₅ OCH ₂ COCH ₃	150.18	6, 151	1.097	1.5210^{20}		230	85	
p75	DL-2-Phenoxy-	CH ₃ CH(OC ₆ H ₅)COOH	166.18	6, 163			116-119	265		s alc; sl s aq
	propionic									

Peracetic acid, p59 Perdeuterocyclohexane, c313 Perylene, d49 Phenacetin, e45 Phenacyl bromide, b221 Phenacyl chloride, c28 9,10-Phenanthraquinone, p62 Phenazone, a309 1,2,4-Phenenyl triacetate, t193 Phenethyl alcohol, p113 sec-Phenethyl alcohol, m138 Phenethylamine, p114 Phenethyl bromide, b283 Phenethyl chloride, c108 p-Phenetidine, e24 Phenetole, e28 Phenoxyacetone, p74 4-Phenoxybutyl bromide, b243

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p76 p76a p77	3-Phenoxytoluene Phenylacetaldehyde 2-(2-Phenyl- acetamido)- acetaldoxime	C ₆ H ₅ OC ₆ H ₄ CH ₃ C ₆ H ₅ CH ₂ CHO C ₆ H ₅ CH ₂ CONHCH ₂ - CH—NOH	184.24 120.15 192.22	6, 377 7, 292	1.051 1.027 ²⁵ 25	1.5727 ²⁰ 1.5273 ²⁰	33–34 147–151	271–273 195	>112 86	sl s aq; s alc, eth
p78 p79 p80 p81	Phenyl acetate Phenylacetic acid Phenylacetonitrile Phenylacetyl chloride	C ₆ H ₃ OOCCH ₃ C ₆ H ₃ CH ₂ COOH C ₆ H ₃ CH ₂ CN C ₆ H ₃ CH ₂ COCl	136.15 136.15 117.15 154.60	6, 152 9, 431 9, 441 9, 436	$ \begin{array}{c} 1.073_4^{20} \\ 1.091_4^{77} \\ 1.0214_{15}^{15} \\ 1.169 \end{array} $	1.5030 ²⁰ 1.5233 ²⁰ 1.5325 ²⁰	76.5 -23.8	196 265.5 233.5 95 ^{12mm}	76 101	misc alc, eth, chl s hot aq, alc, eth i aq; misc alc, eth d aq, alc
p82 p83 p84 p85	Phenylacetylene Phenylacetylurea L-3-Phenyl-α- alanine 2-(Phenylamino)- benzoic acid	$C_6H_5C \equiv CH$ $C_6H_5CH_2CONHCONH_2$ $C_6H_5CH_2CH(NH_2)COOH$ $C_6H_5NHC_6H_4COOH$	102.14 178.19 165.19 213.24	5, 511 14, 495 14, 327	0.930040	1.5470 ²⁰	-44.9 212-216 d 283 185 d	142.4	31	misc alc, eth sl s alc, bz, chl, eth 3 aq; s hot alc; i eth s hot alc
p86	Phenyl 4-amino- salicylate	H ₂ NC ₆ H ₃ (OH)COOC ₆ H ₅	229.24				153			0.7 mg aq
p87 p88	<i>p</i> -Phenylazoaniline Phenylazoformic acid 2-phenylhydrazide	$C_6H_5N = NC_6H_4NH_2$ $C_6H_5N = NCONHNHC_6H_5$	197.24 240.27	16 ¹ , 310 16, 24			128 156– 159 d	>360		v s alc, bz, chl, eth
p89 p90	<i>p</i> -Phenylazophenol 2-Phenylbenzimi- dazole	C ₆ H ₅ N=NC ₆ H ₄ OH	198.23 194.24	16, 96 23, 230			155–157 291	230 ^{20mm}		v s alc, eth s abs alc; sl s bz, chl
p91 p92 p93	Phenyl benzoate N-Phenylbenzylamine 1-Phenylbiguanide	$C_6H_5COOC_6H_5 C_6H_5CH_2NHC_6H_5 C_6H_5NHC(=NH)NH- C(=NH)NH_2$	198.22 183.25 177.21	9, 116 12, 1023	1.235 1.061		70 27–38 144–146	314 306–307		v s hot alc; sl s eth s alc, chl, eth v s aq, alc

p94	1-Phenyl-2-butanone	CH ₃ CH ₂ COCH ₂ C ₆ H ₅	148.21	7, 314	0.998	1.512220		112 ^{15mm}	90	s alc; misc eth; i
p95	4-Phenyl-2-butanone	C ₆ H ₅ CH ₂ CH ₂ COCH ₃	148.21	7, 314	0.989	1.5122^{20}		235	98	s alc, eth
p96	(E)-4-Phenyl-3- buten-2-one	C ₆ H ₅ CH=CHCOCH ₃	146.19	7, 364	1.009745	1.583645	41.5	261	65	v s alc, bz, chl, eth
p97	4-Phenylbutylamine	C ₆ H ₅ CH ₂ CH ₂ CH ₂ - CH ₂ NH ₂	149.24	12, 1165	0.944	1.5196 ²⁰		124 ^{17mm}	101	
p98	2-Phenyl-3-butyn- 2-ol	$CH_3C(OH)(C_6H_5)C \equiv CH$	146.19	$6^2,559$			51–52	217–218		0.8 aq; s alc, bz, acet
p99	2-Phenylbutyric acid	CH ₃ CH ₂ CH(C ₆ H ₅)COOH	164.20	$9^2,356$			42-44	270-272		s bz, eth
p100	4-Phenylbutyric acid	C ₆ H ₅ CH ₂ CH ₂ COOH	164.20	9, 539			50-52	165 ^{10mm}		s alc, eth
p101	DL-2-Phenylbutyro- nitrile	CH ₃ CH ₂ CH(C ₆ H ₅)CN	145.21	9, 541	0.974	1.5086 ²⁰		114– 115 ^{15mm}	>112	
p102	Phenyl chloroformate	C ₆ H ₅ OOCCl	156.57					71 ^{9mm}		
p103	S-Phenyl chlorothio- formate	C₀H₅SCOCl	172.6		1.269 ₄ ³⁰	1.5786 ³⁰	-14	101 ^{10mm}	116	

Phenylacetaldehyde dimethyl acetal, d450

N-Phenylacetamide, a18 Phenylacetone, p144

2-Phenylacetoacetonitrile, a51

 α -Phenylacetophenone, d22

 β -Phenylacrylic acid, c267

γ-Phenylallyl alcohol, c270

o-Phenylanisole, m56

N-Phenylanthranilic acid, p85
Phenylarsonic acid, b11
Phenylazoformic acid 2-phenylhydrazide, d660
N-Phenylbenzamide, b5
Phenylbenzene, b134
Phenylbenzoic acid, b135
p-Phenylbenzyl alcohol, b138
Phenylboric acid, b12

1-Phenylbutane, b423 2-Phenylbutane, b424 1-Phenyl-1,3-butanedione, b64 4-Phenyl-*sec*-butyl acetate, m361 Phenyl Cellosolve, p72 Phenyl chloride, c41

p9(

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p104 p105	Phenylcyclohexane Phenyl dichloro- phosphate	$C_6H_5C_6H_{11}$ $C_6H_5OP(O)Cl_2$	160.26 210.98	5, 503 6, 179	0.9427 ²⁰ 1.412	1.5263 ²⁰ 1.5230 ²⁰	7.0	240.1 241–243	98 >112	v s alc, eth
p106	N-Phenyldiethanol- amine	$C_6H_5N(CH_2CH_2OH)_2$	181.24	12, 183	1.120^{60}_{20}		56–58	350 sl d		5 aq; v s alc; 29 eth; 25 bz
p107	o-Phenylenediamine	$C_6H_4(NH_2)_2$	108.14	13, 6			103-104	256-258		v s alc, chl, eth
p108	<i>m</i> -Phenylethanol	$C_6H_4(NH_2)_2$	108.14	13 ¹ , 10	1.139_{15}^{15}		62-63	234–237		s aq, alc, acet, chl
p109	<i>p</i> -Phenylenediamine	$H_2NC_6H_4NH_2$	108.14	13,61	15		145-147	267	68	1 aq; s alc, chl, eth
p110	o-Phenylene phosphorochloridite	2 0 . 2	174.52	27, 809	1.466	1.571220		80 ^{20mm}	>112	
p111	1-Phenyl-1,2- ethanediol	C ₆ H ₅ CH(OH)CH ₂ OH	138.17	6, 907			66–68	272–274		v s aq, alc, bz, eth, chl, HOAc
p112	1-Phenylethanol	CH ₃ CH(C ₆ H ₅)OH	122.17	6, 475	1.0150_{20}^{20}	1.5211^{20}	21.4	203.9		2.3 aq
p113	2-Phenylethanol	C ₆ H ₅ CH ₂ CH ₂ OH	122.17	6, 478	1.01825	1.5317^{20}	-27	221	102	2 aq; misc alc, eth
p114	2-Phenylethylamine	C ₆ H ₅ CH ₂ CH ₂ NH ₂	212.28	12, 1096	0.9640_4^{25}	1.5332^{20}		195	90	s aq; v s alc, eth
p115	D-(-)-α-Phenyl- glycine	C ₆ H ₅ CH(NH ₂)COOH	151.17	14, 460			305–310			
p116	1-Phenylheptane	$C_6H_5(CH_2)_6CH_3$	176.30	5, 451	0.860	1.484220		233	95	
p117	1-Phenylhexane	$C_6H_5(CH_2)_5CH_3$	162.28	$5^2, 337$	0.861	1.4865^{20}	-61	226	83	misc eth
p118	Phenylhydrazine	C ₆ H ₅ NHNH ₂	108.14	$15^2, 44$	1.0978420	1.6070^{20}	19.5	243.5 d	88	misc alc, bz, chl, eth
p119	Phenyl 3-hydroxy-2- naphthoate	$C_{10}H_6(OH)COOC_6H_5$	264.28	10, 335			129–132	261 ^{160mm}		
p119a	2-Phenyl-2- imidazoline		146.19	23, 154			94–99			
p120	2-Phenylindole		193.25	20, 467			17	250 ^{10mm}		
p121	Phenyl isocyanate	C ₆ H ₅ NCO	119.12	12, 437	1.0956_4^{20}	1.5350^{20}	-30	162–163	55	d aq, alc; s eth
p122	Phenyl isothio-	C ₆ H ₅ NCS	135.19	12, 453	$1.1288_4^{\frac{7}{25}}$	1.649720	-21	221	87	i aq; s alc, eth
-	cyanate									_

p123 p124	N-Phenylmaleimide Phenylmalonic acid	C _s H _s CH(COOH) ₂	173.17 180.16	21,400			89–90 155 d	163 ^{12mm}		s alc, chl, eth
p125	Phenylmercury(II) acetate	C ₆ H ₅ HgOOCCH ₃	336.74				149			0.17 aq; s alc, bz, acet
p126	Phenylmercury(II) chloride	C₀H₅HgCl	313.15				250–252			s bz, eth, pyr
p127	Phenylmercury(II) hydroxide	C ₆ H ₅ HgOH	294.70	16, 952			190 d			
p128	Phenylmethanethiol	C ₆ H ₅ CH ₂ SH	124.21	6, 453	1.058^{20}			194–195	70	
p129	N-Phenylmorpholine		163.22	27, 6			57	268		1.0 aq; v s hot alc
p130	N-Phenyl-1- naphthylamine	$C_{10}H_7NHC_6H_5$	219.29	12, 1224			60–62	226 ^{15mm}		s alc, bz, chl, eth
p130a	1-Phenyloctane	$C_6H_5(CH_2)_7CH_3$	190.33	5, 453	0.8572_4^{20}	1.4840^{20}	-36	261-263	107	misc eth
p131	2-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6^2 , 623	1.213		57	282	123	s alc, chl, eth, alk
p132	4-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6, 674			164–165	305	165	s alc, chl, eth, alk

2-Phenylcinchoninic acid, p149 α-Phenyl-o-cresol, h113 Phenylethane, e68 Phenylethanenitrile, p80 1-Phenylethanol, m138 Phenylethanolamine, a262 N-Phenylethanolamine, a300 Phenylethene, s11 N-Phenylformamide, f31 Phenylglyoxylic acid, b70 Phenylglyoxylonitrile, b68 1-Phenyl-1-hydroxy-2-methylaminopropanes, e1, e2 2,2'-(Phenylimino)diethanol, p106 p-(2-Phenylisopropyl)phenol, m359 Phenyl-\(\alpha\)-methylstyryl ketone, d658 1-Phenylpentane, p54

1.33

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p133	N-phenyl-p-phenyl enediamine	C ₆ H ₅ NHC ₆ H ₄ NH ₂	184.24	13, 76			73–75			
p134	Phenyl <i>N</i> -phenyl- phosphoramido- chloridate	$C_6H_5NHP(=O)(Cl)$ OC_6H_5	267.66	12, 588			132–134			
p135	Phenylphosphinic acid	C ₆ H ₅ PH(O)OH	142.09	16, 791			83–85			
p136	Phenylphosphonic acid	$C_6H_5P(O)(OH)_2$	158.09	16, 803			163–166			
p137	Phenylphosphonic dichloride	C ₆ H ₅ P(O)Cl ₂	194.99	16, 804	1.375	1.5600^{20}	3	258	>112	
p138	Phenylphosphono- thioic dichloride	C ₆ H ₅ P(S)Cl ₂	211.05	16, 807	1.360	1.6244 ²⁰		205 ^{130mm}		
p139	N-Phenylpiperazine		162.24		1.0621_4^{20}	1.5875^{20}		286	>112	i aq; misc alc
p140	2-Phenyl-1,2-	CH ₃ C(C ₆ H ₅)(OH)CH ₂ OH	152.19	6, 930			44–45	160-	>112	
	propanediol							162 ^{26mm}		
p141	3-Phenyl-1-propanol propanethiol	C ₆ H ₅ CH ₂ CH ₂ CH ₂ SH	152.26	6 ¹ , 253	1.010	1.5494 ²⁰		109 ^{10mm}	90	
p142	1-Phenyl-1-propanol	C ₆ H ₅ CH(OH)CH ₂ CH ₃	136.19		0.9915_4^{25}	1.5169^{23}		219		misc alc, bz
p143	3-Phenyl-1-propanol	C ₆ H ₅ CH ₂ CH ₂ CH ₂ OH	136.19	6, 503	1.008	1.5257^{20}	-18	235	109	s aq; misc alc, eth
p144	1-Phenyl-2-propanone	C ₆ H ₅ CH ₂ COCH ₃	134.18	$7^2, 233$	1.0157_4^{20}	1.5160^{20}	27	100 ^{13mm}	84	v s alc, eth; misc bz
p145	2-Phenylpropion- aldehyde	CH ₃ CH(C ₆ H ₅)CHO	134.18	$7^2, 237$	1.009_4^{20}	1.5175^{20}		202–205	69	i aq; s alc
p146	3-Phenylpropionic acid	C ₆ H ₅ CH ₂ CH ₂ COOH	150.18	9, 508	1.047 ₄ ¹⁰⁰		47–48	280		0.6 aq; s bz, alc, chl, eth, HOAc, PE
p147	1-Phenyl-3-pyrazol- idinone		162.19	24, 2			121			10 hot aq; hot alc; s alk, acid

p148 p149	2-Phenylpyridine 2-Phenyl-4- quinolinecarboxylic	$C_6H_5C_5H_4N$	155.20 249.27	20, 424 22, 103		1.6242 ²⁰	214–215	268–270	>112	s alc, eth 0.8 alc; 1 eth; 0.3 chl
p150	acid Phenyl salicylate	C ₆ H ₄ (OH)COOC ₆ H ₅	214.22	10,76	1.25		41–43	173 ^{12mm}		17 alc; 66 bz; s acet, chl, eth;
p151	Phenylselenenyl chloride	C ₆ H ₅ SeCl	191.52	6 ³ , 1110			63–65	120 ^{20mm}		0.015 aq
p152	Phenylsuccinic acid	HOOCCH ₂ - CH(C ₆ H ₅)COOH	194.19	9, 865			167–169	−H ₂ O, >168		s hot aq, alc, eth
p153	S-Phenyl thioacetate	C ₆ H ₅ SCOCH ₃	152.22			1.5720 ²⁰		100 ^{6mm}	79	
p154	1-Phenyl-2- thiourea	C ₆ H ₅ NHC(S)NH ₂	152.22	12, 388	1.3		154			0.25 aq; s alc, alk
p155	Phenyltrichloro- silane	C ₆ H ₅ SiCl ₃	211.56	16, 911	1.32920	1.5230^{20}		201	91	

2-Phenylpropane, i91

3-Phenyl-2-propenoic acid, c267

3-Phenyl-2-propen-1-o1, c270

3-Phenyl-2-propenoyl chloride, c268

3-Phenylpropyl alcohol, p143 Phenyl propyl ketone, b500 $3\hbox{-Phenylpropyl mercaptan, p141}$

Phenyl sulfide, d688 Phenyl sulfone, d689

Phenylsulfonic acid, b22

Phenyl sulfoxide, d690

(Phenylthio)acetic acid, t160

Phenyl thiocarbamide, p154 α-Phenyl-o-toluic acid, b84 Phenyl m-tolyl ether, p76 Phenyl trifluoromethyl ketone, t289

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p156 p157	1-Phenyltridecane Phenyltriethoxy- silane	C ₆ H ₅ (CH ₂) ₁₂ CH ₃ C ₆ H ₅ Si(OC ₂ H ₅) ₃	260.47 240.38	16, 911	0.8555 ²⁰ 0.996	1.4814 ²⁰ 1.4604 ²⁰	10	346 113 ^{1.0mm}	>112 42	
p158	Phenyltrimethoxy-	C ₆ H ₅ Si(OCH ₃) ₃	198.3		1.064_4^{20}	1.4734 ²⁰		211		
p159	Phenyltrimethyl- ammonium bromide	[C ₆ H ₅ N(CH ₃) ₃] ⁺ Br ⁻	216.13	12 ² , 88			210 d			v s aq; s hot alc
p160	Phenyltrimethyl- ammonium chloride	$[C_6H_5N(CH_3)_3]^+Cl^-$	171.67	12, 158			237 subl			s aq; v s alc; sl s chl
p161	Phenyltrimethyl- ammonium iodide	$[C_6H_5N(CH_3)_3]^+I^-$	263.12	$12^2, 88$			175			s aq, alc; sl s acet
p162	Phenyltrimethyl- ammonium tribromide	$C_6H_5N(CH_3)_3]^+Br_3^-$	375.95				114–116			
p163 p164	Phenyltrimethylsilane Phenyltris(tri- methylsiloxy)silane	C ₆ H ₅ Si(CH ₃) ₃ [(CH ₃) ₃ SiO] ₃ SiC ₆ H ₅	150.30 372.8	16 ¹ , 525	$0.873 \\ 0.970_4^{25}$	1.4907 ²⁰ 1.459 ²⁵		168–170 264–266	44 121	
p165	Phenylurea	C ₆ H ₅ NHCONH ₂	136.15	12, 346	1.302		145–147	238		s hot aq, hot alc,
p166	Phenylvinyldi- chlorosilane	$H_2C = CH(C_6H_5)SiCl_2$	203.2		1.196425	1.534 ²⁵		87 ^{1.5mm}		
p167	o-Phthalic acid	$C_6H_4(COOH)_2$	166.13	9, 791	1.593420		206–208			0.6 aq; 10 alc; 0.5 eth; v sl s chl
p168 p169 p170	Phthalic anhydride Phthalide Phthalimide		148.12 134.13 147.13	17, 469 17, 310 21, 458	1.53 1.164 ⁹⁹		130.8 72–74 238	285 subl 290 subl		0.6 aq(d); s alc s alc v s alk; v sl s bz, PE
p171	o-Phthaloyl dichloride	C ₆ H ₄ (COCl) ₂	203.02	9, 805	1.409 ²⁰	1.5684 ²⁰	15–16	280–282	>112	d aq, alc; s eth

p172 p173	Phthalylsulfa- thioazole Picric acid	$(O_2N)_3C_6H_2OH$
p174 p175 p176 p177 p178	Pinane $(+)$ - α -Pinene $(-)$ - β -Pinene α -Pinene oxide β -Pinene oxide	

403.44			
229.11	6, 265	1.76320	
138.3	5, 93	0.839_4^{20}	1.4616^{20}
136.24	5, 146	0.8591_4^{20}	1.4660^{20}
136.24	5, 154	0.8590^{20}	1.4666^{20}
152.24	5, 152	0.964	1.4690^{20}
152.24	$17^2, 44$	0.976	1.4765^{20}

272 d s alk; sl s alc; i chl 122-123 explodes > 300-50167-168 -55155-156 32 32 -61.5166 103^{50mm} 65 100^{27mm} 66

1.3 aq; 8.2 alc; 10 bz; 2.9 chl; 1.6 eth misc alc, eth

Phloroglucinol, t305 Phorone, d529 Phthalaldehydic acid, f33 m-Phthalic acid, b16 p-Phthalic acid, b17 Phthalonitrile, d236

Picolinaldehyde, p251 Picolines, m398, m399, m400 Picolinic acids, p255, p257 Picolinonitrile, c295 Picolylamines, a223, a224 Picramide, t381

Pimelic acid, h8 Pinacol, d491 Pinacolone, d497 Pinacolyl alcohol, d496 3-Pinanol, i83

$$\begin{array}{c|c} \mathsf{HOOC} & \mathsf{O} \\ \vdots \\ \mathsf{C} - \mathsf{N} \\ \mathsf{H} \end{array} \longrightarrow \begin{array}{c} \mathsf{SO}_2 \mathsf{N} \\ \mathsf{N} - \end{array}$$

p172



TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p179 p180	Piperazine 1-Piperazinecarb- aldehyde		86.14 114.15	23, 4	1.107	1.446 ¹¹³ 1.5094 ²⁰	108–110	145–146 97 ^{0.5mm}	109 101	v s aq; 50 alc; i eth
p181	1,4-Piperazinedi- carbonitrile		136.16	231,5			167–170			
p182	3-(1-Piperazinyl)- 1,2-propanediol		160.22				73–77	133 ^{0.1mm}		
p183	Piperidine		85.15	20, 6	0.865915	1.4525^{20}	-10.5	106.4	4	misc aq; s alc, bz,
p184	1-Piperidine- carbonitrile		110.16	20, 56	0.951	1.4705^{20}		102 ^{10mm}	97	
p185 p186 p187	N-Piperidineethanol 2-Piperidineethanol 3-Piperidinemethanol		129.20 129.20 115.18	20, 25 21, 2 21 ² , 8	$ \begin{array}{c} 0.9732_{25}^{25} \\ 1.010^{17} \\ 1.026 \end{array} $	1.4804 ²⁰	38–40	200–202 234 107 ^{3.5mm}	68 102 >112	misc aq; s alc v s aq, alc, eth
p188	1-Piperidinepropio- nitrile		138.21		0.933	1.4695^{20}		111 ^{16mm}		
p189	3-Piperidino-1,2- propanediol		159.23	20, 34	25		77–80			
p190 p191	trans-Piperitol Propane	CH ₃ CH ₂ CH ₃	154.3 44.10	1, 104	$0.9178^{25} \\ 0.5842^{-42}$	1.4729 ²⁰ 1.3397 ⁻⁴²	-187.7	-42.1		6.5 mL aq; 790 mL alc; 926 mL eth; 1300 mL chl; 1450 mL bz
p192	1,2-Propanediamine	CH ₃ CH(NH ₂)CH ₂ NH ₂	74.13	4, 257	0.87815	1.4460^{20}		119.7	33	misc aq, bz; s alc, eth
p193	1,3-Propanediamine	H ₂ NCH ₂ CH ₂ CH ₂ NH ₂	74.13	4, 261	0.884_4^{25}	1.4575^{20}	-12	140	48	misc alc, eth; s aq
p194	1,2-Propanediol	CH ₃ CH(OH)CH ₂ OH	76.10	1,472	1.0364420	1.4331 ²⁰	-60	188	107	misc aq, acet, chl; s alc, eth
p195	1,3-Propanediol	HOCH ₂ CH ₂ CH ₂ OH	76.10	1,475	1.0597_4^{20}	1.4396^{20}	-26.7	214.4	79	misc aq, alc

p196	1,3-Propanedithiol	HSCH ₂ CH ₂ CH ₂ SH	108.23	1,476	1.0772_4^{20}	1.5405^{20}	-79	169	40	misc alc, bz, eth,
p197	1-Propanesulfonyl	CH ₂ CH ₂ CH ₂ SO ₂ Cl	142.60	4, 8	1.2864415			66 ^{8mm}		chl d hot aq, hot alc
p198	1,3-Propane sultone		122.14		1.392		30–33	180 ^{30mm}		

Pipecolines, m369, m370, m371 1-Piperazineethanol, h123 1-Piperidinecarboxyaldehyde, f35 Piperonal, m239 Piperonyl alcohol, m242 Piperonyl butoxide, m243 Piperonylic acid, m241 Pivalaldehyde, d596 Pivalamide, d597 Pivalic acid, d598 Pivalic anhydride, d599 Pivaloyl chloride, d600 Pivaloyloxymethyl chloride, c151 POPOP, b198 PPO, d679

Prehnitene, t97

Procaine, d271
Proline, p273
Propadiene, a78
1-Propanal, p211
1,3-Propanedicarboxylic acid, g11
Propanedioic acid, m3
1,2-Propanediol cyclic carbonate, p225

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p199 p200	1-Propanethiol 2-Propanethiol	CH ₃ CH ₂ CH ₂ SH CH ₃ CH(SH)CH ₃	76.16 76.16	1, 359 1, 367	$0.836_4^{25} \\ 0.809_4^{25}$	$1.4380^{20} 1.4255^{20}$	-113.1 -130.5	67.7 52.6	-20 -34	s alc, eth misc alc, eth; sl s aq
p201	1,2,3-Propanetriol triacetate	H ₃ CCOO- CH(CH ₂ OOCCH ₃) ₂	218.21	2, 147	1.596 ²⁰	1.4302^{20}	-78	258–260	148	7.2 aq; misc alc, bz, chl, eth
p202	1-Propanol	CH ₃ CH ₂ CH ₂ OH	60.10	1,350	0.8037_4^{20}	1.3856^{20}	-126.2	97.2	15	misc aq, alc, eth
p203	2-Propanol	(CH ₃) ₂ CHOH	60.10	1, 360	0.7855_4^{20}	1.3772^{20}	-89.5	82.4	22	misc aq, alc, chl, eth
p204	2-Propenal	H ₂ C=CHCHO	56.07	1,725	0.838920	1.4017^{20}	-87.0	52.7	-18	21 aq; s alc, eth
p205	Propene	H ₂ C=CHCH ₃	42.08	1, 196	0.6104 ₄ ⁻⁴⁸	1.3567 ⁻⁴⁰	-185.2	-47.7		45 mL aq; 1200 mL alc; 500 mL acet
p206	2-Propene-1-thiol	H ₂ C=CHCH ₂ SH	74.15	1,440	0.925_4^{23}			67–68	21	misc alc, eth
p207	(Z)-1,2,3-Propene- tricarboxylic acid		174.11	2, 849			d 200			50 aq; s alc; sl s eth
p208	1-Propen-2-yl acetate	$H_2C = C(OOCCH_3)CH_3$	100.12		0.909	1.4000^{20}		97	18	
p209	o-Propenylphenol	CH ₃ CH=CHC ₆ H ₄ OH	134.18	$6^1,279$	1.044	1.5754^{20}		230-231	90	
p210	β-Propiolactone		72.06		1.1460420	1.4131 ²⁰	-33.4	162.3	70	37 aq(hyd); misc alc (reacts), bz, eth, acet
p211	Propionaldehyde	CH₃CH₂CHO	58.08	1,629	0.8071_4^{20}	1.364619	-81	48–49	-9	30 aq; misc alc, eth
p212	Propionamide	CH ₃ CH ₂ CONH ₂	73.10	2, 243	0.9597_4^{20}	1.4160^{110}	79	222.2		v s aq, alc, chl, eth
p213	Propionic acid	CH₃CH₂COOH	74.09	2, 234	0.9934 ₄ ²⁰	1.3865^{20}	-21	140.8	51	misc aq; s alc, chl, eth
p214	Propionic anhydride	$[CH_3CH_2C(=O)]_2O$	130.14	2, 242	1.0125_4^{20}	1.4047^{20}	-45	167	73	d aq; s alc, chl, eth
p215	Propionitrile	CH ₃ CH ₂ CN	55.08	2, 245	0.7818420	1.3658 ²⁰	-92.8	97.2	6	10 aq; misc alc, eth

p216 p217	Propionyl chloride Propiophenone	CH ₃ CH ₂ COCl C ₆ H ₅ COCH ₂ CH ₃	92.53 134.18	2, 243 7 ² , 231	$\begin{vmatrix} 1.065_4^{20} \\ 1.0105_4^{20} \end{vmatrix}$	$1.4051^{20} \\ 1.5258^{20}$	-94 18.6	80 218.0	11 87	d aq, alc misc bz, eth, abs
p218	Propoxytrimethyl-silane	CH ₃ CH ₂ CH ₂ OSi(CH ₃) ₃	132.3		0.768420	1.38420		100 ^{735mm}		aic
p219	Propyl acetate	CH ₃ CH ₂ CH ₂ OOCCH ₃	102.13	2, 129	0.836_4^{20}	1.3844 ²⁰	-92	101.6	12	2.3 aq; misc alc, eth
p220 p221	Propylamine 2-(Propylamino)- ethanol	CH ₃ CH ₂ CH ₂ NH ₂ C ₃ H ₇ NHCH ₂ CH ₂ OH	59.11 103.17	4, 136 4, 282	0.7173 ²⁰ 0.900	$1.3882^{20} \\ 1.4415^{20}$	-83.0	47.9 182 ^{746mm}	-37 78	misc aq, alc, eth
p222 p223 p224 p225 p226	Propylbenzene Propyl benzoate Propylcyclohexane Propylene carbonate Propyleneimine	CH ₃ CH ₂ CH ₂ C ₆ H ₅ C ₆ H ₅ COOCH ₂ CH ₂ CH ₃ CH ₃ CH ₂ CH ₂ C ₆ H ₁₁	120.20 164.20 126.24 102.09 57.09	5, 390 9, 112 5 ² , 23	$ \begin{vmatrix} 0.8621_4^{20} \\ 1.0232^{20} \\ 0.7929_4^{20} \\ 1.2041_4^{20} \\ 0.8017^{25} \end{vmatrix} $	$1.4912^{20} 1.5003^{20} 1.4370^{20} 1.4210^{20} 1.4084^{25}$	-99.6 -51.6 -94.9 -55	159.2 231.2 156.7 240 66.0	47 132	s alc, eth i aq; s alc, eth s bz, eth v s aq, alc, bz, eth misc aq, alc, PE

1,2,3-Propanetriol, g16 Propanetriol diacetates, g17, g18 2-Propanone, a26 Propargyl alcohol, p242 Propargyl chloride, c232 Propenamide, a62

2-Propenenitrile, a64 2-Propenoic acid, a63 2-Propen-1-o1, a81 2-Propenyl acetate, a80 Propenylanisole, m97 N-2-Propenyl-2-propen-1-amine, d25 (2-Propenyl)thiourea, a101 Propiolic acid, p241 Propyl chloride, c210 Propylene, p205 Propylene dibromide, d92 sec-Propylene chlorohydrin, c213 Propylenediamine, p192 Propylene glycol, p194 Propylene glycol isopropyl ether, i86 Propylene glycol monomethyl ether, m95 Propylene glycol monophenyl ether, p73

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p227	Propylene oxide	CH ₃ CH—CH ₂	58.08	17,6	0.828720	1.3660 ²⁰	-112.1	37–38	-37	41 aq; misc alc, eth
p228	Propylene sulfide	CH ₃ CH—CH ₂	102.18	1,354	0.736	1.3800^{20}	-123	88–90	4	
p229 p230	Propyl formate Propyl 4-hydroxy- benzoate	CH ₃ CH ₂ CH ₂ OOCH HOC ₆ H ₄ COOCH ₂ CH ₂ CH ₃	88.10 180.20	2, 21 10, 160	0.9006420	1.3769 ²⁰	-92.9 86–87	80.9	-3	2 aq; misc alc, eth 0.05 aq; v s alc, eth
p231 p232	Propyl isocyanate Propyl lactate	CH ₃ CH ₂ CH ₂ NCO CH ₃ CH(OH)COOC ₃ H ₇	85.11 132.16	4 ¹ , 366 3, 265	0.908 0.996^{20}_{20}	$1.3970^{20} \\ 1.4167^{25}$		83–84 86 ^{40mm}	26	s aq, alc, eth
p233	Propyl nitrate	CH ₃ CH ₂ CH ₂ ONO ₂	105.09	1, 355	1.0538420	1.3976 ²⁰	-100 may explo	110.1 de on heatin	23 1g	s alc, eth
p234	2-Propylpentanoic acid	(CH ₃ CH ₂ CH ₂) ₂ CHCOOH	144.21	2, 350	0.921	1.4250^{20}		220		
p235	o-Propylphenol	CH ₃ CH ₂ CH ₂ C ₆ H ₄ OH	136.19	6, 499	1.015^{20}	1.5279^{20}		224–226	93	s alc, eth
p236	Propylphosphonic dichloride	CH ₃ CH ₂ CH ₂ P(O)Cl ₂	160.97	4, 596	1.290	1.4643 ²⁰		88–90 ^{50mm}	>112	
p237	Propyltrichloro- silane	CH ₃ CH ₂ CH ₂ SiCl ₃	177.53	4, 630	1.1851 ₄ ²⁰	1.429^{20}		123–124	2	
p238	Propyltriethoxy- silane	$C_3H_7Si(OC_2H_5)_3$	206.4		0.892_4^{20}	1.396^{20}		179–180		
p239	Propyl 3,4,5-tri- hydroxybenzoate	$(HO)_3C_6H_2COOC_3H_7$	212.20				150			0.35 aq; 1 alc; 83 eth
p240	Propyne	СН₃С≡СН	40.06	1, 246	0.691_4^{-20}	1.3725^{-20}	-102.8	-23.2		v s alc; 3000 mL eth
p241	2-Propynoic acid	НС≡ССООН	70.05	2, 477	1.138_4^{20}	1.4320^{20}	9	102 ^{200mm}	58	s aq, alc, eth
p242	2-Propyn-1-ol	HC≡CCH ₂ OH	56.06	1, 454	0.9715_4^{20}	1.4320^{20}	-51.8	113.6	33	misc aq, alc, bz,
p243	(+)-Pulegone		152.24	7, 81	0.9346_4^{15}	1.4850^{20}		224	82	misc alc, chl, eth

p244	Pyrazine		80.09	23, 91	1.031_4^{61}	1.4953 ⁶¹	53	115–116		v s aq, alc, eth
p245	Pyrazole		68.08	23, 39		1.4203	70	186–188		s aq, alc, bz, eth
p246	Pyrene		202.26	5, 693			150-151			
p247	Pyridazine		80.09	23, 89	1.1035_4^{25}	1.5230 ²³	-8	208	85	misc aq, bz; v s alc, eth
p248	Pyridine	C ₅ H ₅ N	79.10	20, 181	0.9782_4^{25}	1.506725	-41.6	115.2	20	misc aq, alc, eth
p249	Pyridine-d ₅	C_5D_5N	84.14		1.05	1.5079^{20}		114.4	20	_
p250	2-Pyridinealdoxime	$(C_5H_4N)CH = NOH$	122.13	211, 288			110-112			
p251	2-Pyridinecarb-	(C ₅ H ₄ N)CHO	107.11	211, 287	1.126	1.5370^{20}		181	54	
	aldehyde									
p252	3-Pyridinecarb-	(C₅H₄N)CHO	107.11	21 ¹ , 288	1.135	1.5493^{20}		97 ^{15mm}	60	
	aldehyde									
p253	4-Pyridinecarb- aldehyde	(C ₅ H ₄ N)CHO	107.11	21, 287	1.172	1.5440 ²⁰		78 ^{12mm}	54	s aq, eth
p254	3-Pyridinecarbamide	(C ₅ H ₄ N)CONH ₂	122.13	22, 40	1.400	1.466	130-133			100 aq; 66 alc
p255	Pyridine-2-car- boxylic acid	(C ₅ H ₄ N)COOH	123.11	22, 33			134–136	subl		s aq, alc, bz
p256	Pyridine-3-car- boxylic acid	(C ₅ H ₄ N)COOH	123.11	22, 38	1.473		236.6	subl		1.4 aq; s alk

Propylene oxide, e10 Propyl gallate, p239 Propyl iodide, i48 Propyl mercaptan, p199 6-Propyl-2-thiouracil, h129 Protocatechualdehyde, d376 Pseudocumene, t334 Pyrene, b52

3,6-Pyridazinediol, d400 2.3-Pyridinediol, d401

p244

p245

p247

.349

TABLE 1.15 Physical Constants of Organic Compounds (continued)

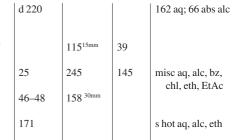
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p257	Pyridine-4-car-	(C ₅ H ₄ N)COOH	123.11	22, 45			319	260 ^{15mm}		0.52 aq; i alc, bz,
p258	boxylic acid 4-Pyridinecar- boxylic hydrazide	(C ₅ H ₄ N)CONHNH ₂	137.14	22 ¹ , 504			171.4			eth 14 aq; 2 alc; 0.1 chl
p259	2,3-Pyridinedi- carboxylic acid	$(C_5H_3N)(COOH)_2$	167.12	22, 150			190 d			0.56 aq; s alk
p260	2,5-Pyridinedi- carboxylic acid	$(C_5H_3N)(COOH)_2$	167.12	22, 153			236–237	subl d		s hot acid
p261	2,6-Pyridinedi- carboxylic acid	(C ₅ H ₃ N)(COOH) ₂	167.12	22, 154			250 d			sl s aq; v sl s alc
p262	Pyridine-N-oxide	$C_5H_5N(O)$	95.10	20 ² , 131			66	270		
p263	3-Pyridinesulfonic acid	(C ₅ H ₄ N)SO ₃ H	159.16	22, 387			>300			v s aq
p264	2-Pyridylmethanol	(C ₅ H ₄ N)CH ₂ OH	109.13	21 ¹ , 203	1.131	1.5420^{20}		113 ^{16mm}		v s aq, alc, eth
p265	3-Pyridylmethanol	(C ₅ H ₄ N)CH ₂ OH	109.13	21,50	1.124	1.5445^{20}		154 ^{28mm}		v s aq, eth
p266	3-(3-Pyridyl)-1- propanol	(C ₅ H ₄ N)CH ₂ CH ₂ CH ₂ OH	137.18	,	1.045	1.5295 ²⁰				P
p267	Pyrimidine		80.09	23, 89	1.016	1.5035^{20}	20-22	123-124	31	misc aq; s alc, eth
p268	2,4(1H,3H)-Pyrimi- dinedione		112.09	24, 312			335			0.3 aq; s alk
p269	Pyrrole		67.09	20, 159	0.9691_4^{20}	1.5102^{20}	-23.4	129.8	38	4.5 aq; v s alc, eth
p270	Pyrrolidine		71.12	20, 4	0.8520_4^{22}	1.4431 ²⁰	-57.8	88–89	2	misc aq; s alc, chl,
p271	1-Pyrrolidinecarbo- dithioic acid, ammonium salt		164.29				153–155			
p272	1-Pyrrolidinecarbo- nitrile		96.13		0.954	1.4690 ²⁰		77 ^{1.8mm}	107	

p273	L-(-)-2-Pyrrol- idinecarboxylic acid
p274	1-Pyrrolidino-1- cyclohexene
p275	2-Pyrrolidinone
p276 q1	3-(N-Pyrrolidino)- 1,2-propanediol Quinhydrone
•	

Pyridinols, h173, h174, h175 3-Pyridinol *N*-oxide, h177 2(1*H*)-Pyridone, h173 2-(2-Pyridyl)pyridine, d705 Pyrocatechol, d377

115.13	22, 2		
151.25		0.940	1.5225 ²⁰
85.11	21, 236	1.116425	1.486 ²⁵
145.20	201, 4		
218.20	7,617	1.401420	

Pyrogallol, t304 Pyromellitic acid, b26 Pyromellitic dianhydride, b27 Pyromucic acid, f42 Pyromucic aldehyde, f39



Pyrrolidinedithiocarbamate, p271 Pyruvic acid, o60 Pyruvic aldehyde, o59 Pyruvic aldehyde dimethyl acetal, d451 Quinaldine,

CH₂CHOHCH₂OH

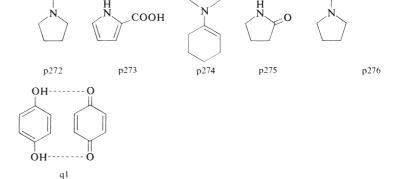


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
q2	Quinine		324.44			1.625	177 d			125 alc; 1.2 bz; 83 chl
q3	Quinoline		129.16	20, 339	1.095_4^{20}	1.6273 ²⁰	-14.9	237	101	0.6 aq; misc alc, eth
q4 q5	Quinoxaline Quinuclidine		130.15 111.19	23, 176 20, 144	1.133448	1.623148	29–30 156	229.5		v s aq, alc, bz, eth v s aq, alc, eth
							sealed tube			
r1	D-Raffinose pentahydrate		594.52	31, 462			80	d 118		14 aq; 10 MeOH
r2	Rhodamine B		479.02	19, 346			165			v s aq, alc
r3	Rhodanine		133.19	27, 242	0.868		170			v s hot aq, alc, eth
							may explo	de on rapid	heating	
r4	Riboflavin		376.37				d 278			v s alk(d); i eth
r5	D-(-)-Ribose		150.13	11, 434			87			s aq; sl s alc
s1	Saccharin		183.19	27, 168			229–230			0.34 aq; 3 alc; 8
										acet
s2	Safrole		162.19	19, 39	1.095 ²⁰	1.5370^{20}	11.2	232–234	97	v s alc; misc chl eth
s3	Semicarbazide	H ₂ NNHCONH ₂	75.07	3,98			96			v s aq, alc; i eth

Quinizarin, d372 Quinolinic acid, p259 8-Quinolinol, h178 p-Quinone, b59 Resacetophenone, d370 Resorcinol, d378 Resorcinol dimethyl ether, d432 Resorcinol monoacetate, d380 Resorcinol sulfide, t145 $\alpha\textsc{-Resorcylaldehyde, d375}$ $\alpha\textsc{-Resorcylic acid, d385}$ $\beta\textsc{-Resorcylic acid, d383}$ Ribofuranose, r5 Rosaniline, b2 Rubeanic acid, d710 Slicyl alcohol, h105 Salicylaldehyde, h94 Salicylaldoxime, h97

Salicylamide, h98 Salicylanilide, h161 Salicylic acid, h99 Salol, p150 Sarcosine, m258 Sebacic acid, d9 Sebacoyl chloride, d11 Semioxamazide, 053

$$CH_{2}=CH$$

$$H$$

$$HO$$

$$H$$

$$Q^{2}$$

$$CI^{-}$$

$$N(C_{2}H_{5})_{2}N$$

$$COOH$$

$$T^{2}$$

$$T^{2}$$

ÇH₂OH

HOĊH

HOCH

носн

r4

ĊH₂

O

q4

CH₃

CH₃

CH₂CH=CH₂

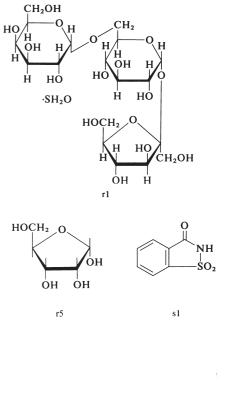


TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
s4 s5	L-Serine D-Sorbitol	HOCH ₂ CH(NH ₂)COOH	105.09 182.17	4, 505 1, 533	1.472 ⁻⁵		222 d 110–112			s aq; v sl s alc, eth 83 aq; s hot alc, acet
s6	L-(-)-Sorbose		180.16	1,927	1.6515		165			55 aq; v sl s alc
s7	Squalane	[(CH ₃) ₂ CH(CH ₂) ₃ - CH(CH ₃)(CH ₂) ₃ - CH(CH ₃)CH ₂ CH ₂ -] ₂	422.80	1 ¹ , 72	0.810	1.453015	-38	350	218	s bz, chl, eth, PE
s8	Squalene	$ \begin{cases} CH_3[C(CH_3) = CHCH_2 - CH_2]_2C(CH_3) = CHCH_2 - CHCH_2 \end{cases} $	410.73	11, 130	0.8584_4^{20}	1.4965 ²⁰	-75	285 ^{25mm}	200	v s eth, acet, PE
s9	trans-Stilbene	C ₆ H ₅ CH=CHC ₆ H ₅	180.25	5,630	0.970		124	206-207		v s bz, eth
s10	L-Strychnine		334.42	27 ² , 723	1.36420		284–286	270 ^{5mm}		6.2 alc; 20 chl; 0.55 bz; 15 mg
s11	Styrene	C ₆ H ₅ CH=CH ₂	104.15	5, 474	0.9060^{20}	1.5468 ²⁰	-30.6	145.1	31	s alc, acet, eth
s11	Succinamic acid	H,NCOCH,CH,COOH	117.10	2,614	0.9000	1.5406	153–156	143.1	31	s ac; acet, eur
s12	Succinamide Succinamide	H ₂ NCOCH ₂ CH ₂ COOH ₂	116.12	2,614			260 d	125 subl		0.45 aq; i alc, eth
s14	Succinic acid	HOOCCH,CH,COOH	118.09	2,601	1.552		187–190	235 d		7.7 aq; 5.4 alc; 2.8
511	Succime acid		110.07	2,001	1.332		107 170	233 4		acet; 0.88 eth; i
s15	Succinic acid 2,2- dimethylhydrazide	HOOCCH ₂ CH ₂ CONH- N(CH ₃) ₂	160.17				154–155			11 aq; 2.5 acet; 5 MeOH
s16	Succinic anhydride	3/2	100.07	17, 407			119.6	261		s alc, chl; v sl s eth
s17	Succinimide		99.09	21, 369	1.41		125-127	287		33 aq; 4 alc; i eth
s18	Succinonitrile	NCCH ₂ CH ₂ CN	80.09	2,615	0.985		46-48	265-267	>112	•
s19	Succinyl chloride	CICOCH ₂ CH ₂ COCl	154.98	2,613	1.395_4^{15}	1.47315	17	192-193	76	d aq, alc; s bz
s20	Sucrose		342.30	31, 424	1.587_4^{25}		192 d			200 aq; 0.59 alc
s21	Sulfamethazine		278.34				198-201			0.15 aq; s alk
s22	Sulfanilamide	H ₂ NC ₆ H ₄ SO ₂ NH ₂	172.21	14, 698			164–166			0.76 aq; 2.7 alc; 20 acet; s acid, alk

s23 s24	Sulfoacetic acid o-Sulfobenzoic acid	HO ₃ SCH ₂ COOH	140.11 184.17	4, 21 19, 110		84–86	245 d 186 ^{18mm}	s aq, alc; i eth, chl s bz, chl, eth; i aq
s25	cyclic anhydride 4,4'-Sulfonylbis- (2,6-dibromo- phenol)	$[HO(Br)_2C_6H_2]_2SO_2$	565.88	6, 865		289–292		

Senecioic acid, m163 Skatole, m284 Sodium tetraphenylborate, t128 Solketal, d515 Sorbic acid, h42 Sorbic aldehyde, h40 Stearamide, o2 Stearic acid, o5 Stearyl bromide, b319 Styrene dibromide, d79 Styrene glycol, p111 Styrene oxide, e9 Suberic acid, o24 Suberonitrile, d239 Succinic acid monoamide, s12 Succinonitrile, b380 Succinyl dihydrazide, s15 Sulfanilic acid, a120 N-Sulfinylaniline, t152 3-Sulfoalanine, a288 Sulfolane, t106 3-Solfolene, d368 Sulfonyldianilines, d36, d37

$$H_2N - \underbrace{\hspace{1cm} \begin{array}{c} CH_3 \\ N - \\ N - \\ CH_3 \end{array}}_{CH_3}$$

s21

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
s26	4,4'-Sulfonylbis-	(CH ₃ OOCC ₆ H ₄) ₂ SO ₂	334.35	10 ² , 109			195–196			
s27	(methyl benzoate) 4,4'-Sulfonyl- diphenol	(HOC ₆ H ₄) ₂ SO ₂	250.27	6, 861	1.366315		245–247			s alc, eth, acet; i
s28	5-Sulfosalicyclic acid	HO ₃ SC ₆ H ₃ (OH)COOH	254.21	11,411			120			v s aq, alc; s eth
t1	D-(-)-Tartaric		150.09	3, 520	1.7598 ₄ ²⁰		168–170			139 aq; 33 alc; 0.4 eth
t2	meso-Tartaric acid hydrate	HOOCCH(OH)- CH(OH)COOH xH ₂ O	150.09	3, 528	1.666420		140			125 aq
t3	Tartrazine	_	534.37	25, 252						v s aq
t4	p-Terphenyl	$C_6H_5C_6H_4C_6H_5$	230.31	5, 695			212-213	383		_
t5	α-Terpinene		136.24	5, 126	0.8375_4^{20}	1.477520		174	46	misc alc, eth
t6	γ-Terpinene		136.24	5, 128	0.853_4^{15}	1.475416		183	51	
t7	Terpinen-4-ol		154.25	6, 55	0.9338_4^{20}	1.4820^{20}	36.4	219	79	v s alc, eth
t8	Tetraallyloxysilane	(H ₂ C=CHCH ₂ O) ₄ Si	256.4		0.9824_4^{20}	1.4336^{20}		114 ^{12mm}		
t9	1,1,2,2,-Tetrabromo- ethane	Br ₂ CHCHBr ₂	345.67	1,94	2.9529 ²⁵	1.6323 ²⁵	0.0	243.5	none	misc alc, eth; 0.07
t10	Tetrabromophthalic anhydride		463.72	17, 485			274–276			sl s bz; i aq, alc
t11	$\alpha, \alpha, \alpha', \alpha'$ -Tetrabromo- ρ -xylene	$C_6H_4(CHBr_2)_2$	421.77	5, 367			114–116			v s chl
t12	$\alpha,\alpha,\alpha',\alpha'$ -Tetrabromo- <i>m</i> -xylene	$C_6H_4(CHBr_2)_2$	421.77	5, 375			105–108			v s bz, chl
t13	Tetrabutoxysilane	(C ₄ H ₉ O) ₄ Si	320.5		0.899_4^{20}	1.41320		115 ^{3mm}		
t14	Tetrabutylammonium bromide	$(C_4H_9)_4N^+Br^-$	322.38		0.0334	11110	103–104			
t15	Tetrabutylammonium chloride	$(C_4H_9)_4N^+CI^-$	277.92	4 ³ , 292			83–86			

t16	Tetrabutylammonium	$(C_4H_9)_4N^+F^-\cdot 3H_2O$	315.52	$4^3, 292$			62–63			
	fluoride trihydrate									
t17	Tetrabutylammonium	$(C_4H_9)_4N^+HSO_4^-$	339.54				169–171			
	hydrogen sulfate									
t18	Tetrabutylammonium	$(C_4H_9)_4N^+I^-$	369.38	4, 157			145-148			sl s aq; s alc, eth
	iodide									_
t19	Tetrabutylammonium	$(C_4H_9)_4N^+BF_4^-$	329.28	$4^3, 293$			160-162			
	tetrafluoroborate									
t20	Tetrabutyltin	$(C_4H_9)_4Sn$	347.15		1.057	1.4742^{20}	-97	145 ^{10mm}	107	
t21	1,1,3,3-Tetrachloro-	Cl ₂ CHCOCHCl ₂	195.86	1,656	1.624_4^{15}	1.497^{18}		182 ^{745mm}	none	v s acet, chl
	acetone									
t22	1,2,3,4-Tetrachloro-	$C_6H_2Cl_4$	215.89	5, 204			46-47	254	>112	v s eth; sl s alc
	benzene	3 2 .								
t23	1,2,4,5-Tetrachloro-	$C_6H_2Cl_4$	215.89	5, 205	1.85822		138-140	240-246	>112	s bz, chl, eth
	benzene									

Sylvan, m252 Sylvic acid, a1 2,4,5-T, t242 TAPS, t427 Taurine, a161 Terephthaldehyde, b13 Terephthaldicarboxaldehyde, b13 Terephthalic acid, b17

Terephthaloyl chloride, b15 TES, t424 Tetracene, b7

 CH_3

2 7 7

t3

t7

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t24	Tetrachloro-o-	$C_6Cl_4(=O)_2$	245.88	7, 602			127–129			
t25	benzoquinone Tetrachloro-p- benzoquinone	$C_6Cl_4(=O)_2$	245.88	7, 602			290	subl		s eth; sl s chl; i aq
t26	Tetrachloro-1,2- difluoroethane	Cl ₂ CFCFCl ₂	203.83		1.6447 ²⁵	1.4130 ²⁵	26.0	92.8		0.012 aq
t27	1,1,1,2-Tetrachloro- ethane	ClCH ₂ CCl ₃	167.85	1,86	1.598	1.4819 ²⁰		130	none	0.02 aq; misc alc
t28	1,1,2,2-Tetrachloro- ethane	Cl ₂ CHCHCl ₂	167.85	1,86	1.586625	1.4910 ²⁵	-43.8	146.3	none	0.3 aq; misc alc, chl, eth, PE
t29	Tetrachloroethylene	Cl ₂ C=CCl ₂	165.83	1, 187	1.6230_4^{20}	1.5057 ²⁰	-22.4	121.1	none	misc alc, chl, eth
t30	2,3,5-Tetrachloro- nitrobenzene	HC ₆ Cl ₄ NO ₂	260.89	5, 247	1.744 ₄ ²⁵		98–101	304		s alc, bz, chl
t31	Tetrachlorophthalic anhydride		285.90	17, 484			254–258	371		d hot aq; sl s eth
t32	3,4,5,6-Tetrachloro- phthalimide		284.91	21,505			>300			
t33	1,1,2,3-Tetrachloro- 2-propene	CICH=C(Cl)CHCl ₂	179.86	11,83	1.530	1.5163 ²⁰	165		none	
t34	2,3,5,6-Tetrachloro- thioanisole	HC ₆ Cl ₄ SCH ₃	262.0				59–61			
t35	2,4,5,6-Tetrachloro- <i>m</i> -xylene	C ₆ Cl ₄ (CH ₃) ₂	243.95	5, 373			220–222			
t36	Tetracosane	CH ₃ (CH ₂) ₂₂ CH ₃	338.66	1, 175	0.7786^{51}	1.428370	51.1	391		9.4 chl; s eth
t37	Tetracyanoethylene	$(NC)_2C = C(CN)_2$	128.09				200	subl 120		
t38	Tetradecane	CH ₃ (CH ₂) ₁₂ CH ₃	198.40	1, 171	0.7627_4^{20}	1.4290^{20}	5.9	253.5		v s alc, eth
t39	Tetradecanoic acid	CH ₃ (CH ₂) ₁₂ COOH	228.38	2, 365	0.8528470	1.4273 ⁷⁰	58.5	250 ^{100mm}		v s bz, chl, eth; s alc

+40	1 7-4-11	CH (CH) OH	21420	1 420	0.815150	1.435850	27.0	1264	I	l4111-
t40	1-Tetradecanol	CH ₃ (CH ₂) ₁₃ OH	214.39	1,428	0.8151	1.4338	37.8	264		s eth; sl s alc
t41	Tetradecanoyl chloride	CH ₃ (CH ₂) ₁₂ COCl	246.82	2, 368			-1	168 ^{15mm}		d aq, alc; s eth
t42	1-Tetradecene	$CH_3(CH_2)_{11}CH = CH_2$	196.38	1,226	0.775^{15}_{4}	1.4351^{20}	-12.9	251.2	115	v s alc; s eth
t43	7-Tetradecene	$CH_3(CH_2)_5CH$ = CH - $(CH_2)_5CH_3$	196.38		0.764	1.4351 ²⁰		250	99	, ,
t44	1-Tetradecylamine	CH ₃ (CH ₂) ₁₃ NH ₂	213.41	4, 201			40-42	162 ^{15mm}		
t45	4-Tetradecylaniline	CH ₃ (CH ₂) ₁₃ C ₆ H ₄ NH ₂	213.41	$12^3, 2780$			46-49			
t46	Tetradecyltrichloro- silane	CH ₃ (CH ₂) ₁₃ SiCl ₃	331.8	,		1.382		156 ^{3mm}		
t47	Tetraethoxysilane	(CH ₃ CH ₂ O) ₄ Si	208.33		0.934_4^{20}	1.383^{20}	-77	165.8	46	d aq; s alc
t48	Tetraethylammonium bromide	(CH ₃ CH ₂) ₄ N ⁺ Br ⁻	210.16	4, 104	1.3974		287 d			v s aq, alc, acet, chl
t49	Tetraethylammonium chloride	(CH ₃ CH ₂) ₄ N ⁺ Cl ⁻	165.71	4, 104	1.080141		37.5			141 aq; s alc; 8.2 chl
t50	Tetraethylammonium hydroxide	$(CH_3CH_2)_4N^+OH^-$	147.26	4, 103						misc aq
t51	Tetraethylene glycol	(HOCH ₂ CH ₂ OCH ₂ - CH ₂) ₂ O	194.23	1,468	1.125_{20}^{20}	1.4590^{20}	-6	307.8	176	misc aq, alc, bz, eth
t52	Tetraethylene glycol dimethacrylate	[H ₂ C=C(CH ₃)COOCH ₂ CH ₂ OCH ₂ CH ₂] ₂ O	330.37		1.08			220 ^{1mm}	62	
t53	Tetraethylene glycol monomethyl ether	CH ₃ O(CH ₂ CH ₂ O) ₃ CH ₂ CH ₂ OH	208.26		0.987	1.4453 ²⁰		166 ^{11mm}	>112	

Tetraethyl orthosilicate, t47

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t54	Tetraethylenepent- amine	(H ₂ NCH ₂ CH ₂ NHCH ₂ - CH ₂) ₂ NH	189.31		0.999_{20}^{20}	1.5055 ²⁰	-40	340	185	misc aq, alc, eth
t55	N,N,N',N'-Tetra ethylethylene- diamine	(C ₂ H ₅) ₂ NCH ₂ CH ₂ - N(C ₂ H ₅) ₂	172.32	4, 251	0.808	1.4343 ²⁰		189–192	58	
t56	Tetraethylgermanium	(C ₂ H ₅) ₄ Ge	188.84	4,631	1.1989		-90	165.5		s alc, eth; i aq
t57	Tetraethyllead	$(C_2H_5)_a$ Pb	323.45	4, 639	1.65320	1.5198^{20}	-136	152 ^{291mm}		s bz; misc eth
t58	Tetraethyl pyrophosphate	$[(C_2H_5O)_2P(O)]_2O$	290.20		1.185_4^{20}	1.4196^{20}	d 170			d aq; misc alc, bz, chl
t59	Tetraethyl pyrophosphite	$[(C_2H_5O)_2P]_2O$	258.19		1.057	1.434120		81 ^{1mm}	>112	
t60	Tetraethylsilane	(C ₂ H ₅) ₄ Si	144.34	4^2 , 1007	0.762_4^{20}	1.4246^{20}		153–155		i aq
t61	Tetraethylthiuram disulfide	$\left[(C_2H_5)_2NC(=S)S - \right]_2$	296.54	4, 122	1.30		70			3.8 alc; 7.1 eth; s bz, acet, chl; 0.02 aq
t62	Tetraethyltin	$(C_2H_5)_4Sn$	234.94	4,632	1.199_4^{20}		-112	181		i aq; s eth
t63	Tetrafluoroethylene	$F_2C = CF_2$	100.02	1 ³ , 638	1.1507-40		-131.2	-75.6		i aq
t64	2,2,3,3-Tetrafluoro- 1-propanol	HCF ₂ CF ₂ CH ₂ OH	132.06		1.4853 ₄ ²⁰	1.3197^{20}	-15	109–110	49	*
t65	1,2,3,6-Tetrahydro- benzaldehyde	C ₆ H ₉ CHO	110.16	71, 48	0.940	1.4745^{20}		163–164	57	
t66	Tetrahydrofuran		72.11	17, 10	0.8892_4^{20}	1.4072^{20}	-108.5	66	-17	misc aq, alc eth, PE
t67	2,5-Tetrahydrofuran- dimethanol		132.16		1.1542_4^{25}	1.4766 ²⁵	<-50	265		misc aq, alc, bz, chl; s eth
t68	Tetrahydro-2-furan- methanol		102.13	17 ² , 106	1.0524 ²⁰	1.4520^{20}	<-80	178	83	misc aq, alc, bz, chl, eth, acet
t69	Tetrahydro-2-furan- methylamine		101.15	18 ² , 415	0.980	1.4560 ²⁰		154 ^{744mm}	45	

t70	2-(Tetrahydrofuryl- oxy)tetrahydro- pyran		186.25		1.030	1.4606 ²⁰			97	
t71	1,2,3,4-Tetrahydro- isoquinoline		133.19	20, 275	1.064	1.5668 ²⁰	-30	232–233	98	
t72	Tetrahydrolinalool	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ - C(CH ₃)(OH)CH ₂ CH ₃	158.28		0.925^{25}	1.433 ²⁰				
t73	1,2,3,4-Tetrahydro- naphthalene	$C_{10}H_{12}$	132.21	5, 491	0.9702_4^{20}	1.5414 ²⁰	-35.8	207.6	77	misc alc, bz, chl, eth, acet, PE
t74	cis-1,2,3,6-Tetra- hydrophthalic anhydride		152.15	17, 462			101–102			
t75	cis-1,2,3,6-Tetra- hydrophthalimide		151.17				134–138			
t76	Tetrahydropyran		86.14		0.8814_4^{20}	1.4211^{20}	-45	88	-20	misc aq, alc, eth
t77	Tetrahydropyran- 2-methanol		116.16		1.0254 ²⁰	1.4580 ²⁰	−70 glass	187	93	misc aq, alc, bz, eth

Tetraglyme, b190 1,2,3,4-Tetrahydrobenzene, c330 Tetrahydrodicyclopentadiene, t253 Tetrahydro-2,5-dimethoxyfuran, d457 Tetrahydrofurfurylamine, t69 Tetrahydrofurfuryl alcohol, t68

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t78	1,2,3,6-Tetrahydro-		83.13	20³, 1912	0.911	1.4800 ²⁰	-48	108	16	
t79	pyridine 3,4,5,6-Tetrahydro- pyrimidinethiol		116.19	24, 5			210–212			
t80	1,2,3,4-Tetrahydro- quinoline		133.19	20, 262	1.061	1.5924	15–16	249	100	s aq; misc alc, eth
t81	Tetrahydrothiophene		88.17	17 ¹ , 5	0.9987^{20}	1.504820	-96.2	120.9	12	misc alc, eth; i aq
t82	1,4,9,10-Tetra-		242.23	8, 431			147–149			
	hydroxyanthracene									
t83	2,2',4,4'-Tetra-	$[(HO)_2C_6H_3]_2C=O$	246.22	8, 496			200–203			
	hydroxybenzo- phenone									
t84	Tetrahydroxyhexane-	HOOC[CH(OH)],COOH	210.14	3, 581			230 d			0.003 aq; s alk
	dioic acid									1.
t85	Tetrakis(2-ethyl-	[CH ₃ CH ₂ CH(C ₂ H ₅)-	432.8		0.892_4^{20}	1.430^{20}		171 ^{2mm}		
	butoxy)silane	CH ₂ O] ₄ Si								
t86	Tetrakis(2-ethyl-	[CH3(CH2)3CH(C2H5)-	549.95		0.880_4^{20}	1.438820		194 ^{1mm}	190	
	hexoxy)silane	CH ₂ O] ₄ Si								
t87	N,N,N',N'-Tetra-	{[CH ₃ CH(OH)CH ₂] ₂ -	292.42	4 ⁴ , 1685	1.013	1.481220		175-		
	kis(p-hydroxy-	NCH_2-}_2						181 ^{0.8mm}		
	propyl)ethylene diamine									
t88	Tetrakis(isoprop-	[(CH ₃) ₂ CHO] ₄ Si	264.4		0.877_4^{20}	1.38520		64 ^{5mm}		
100	oxy)silane	[(C113)2C110]451	204.4		0.0774	1.505		04		
t89	Tetrakis(2-methoxy-	(CH ₃ OCH ₂ CH ₂ O) ₄ Si	328.4		1.079_4^{20}	1.422^{20}		182 ^{10mm}		
	ethoxy)silane	(- 3 2 - 2 - 74-			4					
t90	Tetrakis(trimethyl-	[(CH ₃) ₃ SiO] ₄ Ti	404.7		0.900_4^{20}	1.42720		110 ^{10mm}		
	siloxy)titanium									

t91	1,1,3,3-Tetramethoxy- propane	[(CH ₃ O) ₂ CH] ₂ CH ₂	164.20		0.997	1.4081^{20}		183	54	
t92	Tetramethoxysilane	(CH ₃ O) ₄ Si	152.2	1, 287	1.052_4^{20}	1.368^{20}		121-122	20	
t93	Tetramethyl- ammonium bromide	$(CH_3)_4N^+Br^-$	154.06	4, 51	1.56		d > 230	subl > 360		55 aq
t94	Tetramethyl- ammonium chloride	$(CH_3)_4N^+Cl^-$	109.60	4, 51	1.16940		d>230	subl > 300		s aq, hot alc
t95	Tetramethyl- ammonium iodide	$(CH_3)_4N^+I^-$	201.06		1.829		d 230			sl s aq; v s abs alc
t96	N,N,3,5-Tetra- methylaniline	$(CH_3)_2C_6H_3N(CH_3)_2$	149.24	12, 1131	0.913	1.5443 ²⁰		226–228	90	
t97	1,2,3,4-Tetramethylbenzene	$C_6H_2(CH_3)_4$	134.22	5, 430	0.905_4^{20}	1.5187 ²⁰	-6.2	205.0	68	misc alc, eth
t98	1,2,3,5-Tetramethylbenzene	$C_6H_2(CH_3)_4$	134.22	5, 430	0.8906_4^{20}	1.5134^{20}	-23.7	198.0	63	s alc; v s eth
t99	1,2,4,5-Tetramethylbenzene	$C_6H_2(CH_3)_4$	134.22	5, 431	0.838481		79.2	196.8	73	v s alc, bz, eth

6,7,8,9-Tetrahydro-5*H*-tetrazoloazepine, p26 Tetrahydrothiophene 1,1-dioxide, t106 Tetrahydrothiophene oxide, t107 Tetrahydroxyadipic acid, t84 Tetralin, t73 β -Tetralonehydantoin, b40

N,N,N',N'-Tetramethyldiaminomethane, t
113 N,N,N',N'-Tetramethyl-1,3-diamino-2-propanol, b
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TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t100	2,2,3,3-Tetramethyl- butane	(CH ₃) ₃ CC(CH ₃) ₃	114.23	1, 165	0.656^{-120}		-120.7	106.5	<1	
t101	N,N,N',N'-Tetra- methyl-1,4-butane- diamine	(CH ₃) ₂ N(CH ₂) ₄ - N(CH ₃) ₂	144.26	4, 265	0.786 ²⁰	1.4280 ²⁰		169	46	s aq, alc, eth
t102	1,1,3,3-Tetramethyl- butylamine	(CH ₃) ₃ CCH ₂ - C(CH ₃) ₂ NH ₂	129.25	4, 198	0.805	1.4240^{20}		137–143	32	s alc, eth, PE; i aq
t103	1,3,5,7-Tetramethyl- cyclotetrasiloxane	[—SiH(CH ₃)O—] ₄	240.5		0.9912_4^{20}	1.3870^{20}	-69	134–135		
t104	1,1,4,4-Tetramethyl- 1,4-dichlorodisilyl- ethylene	[(CH ₃) ₂ Si(Cl)CH ₂ —] ₂	215.3				37	198 ^{734mm}	68	
t105	Tetramethyldi- siloxane	[(CH ₃) ₂ SiH] ₂ O	134.3		0.757_4^{20}	1.37020		71 ^{731mm}		
t106	Tetramethylene sulfone		120.71	17 ¹ , 5	1.2614 ₄ ³⁰	1.482030	27.6	285	165	misc aq, acet, bz
t107	Tetramethylene sulfoxide		104.17		1.158	1.5200^{20}			>112	
t108	N,N,N',N'-Tetra- methylethylene diamine	(CH ₃) ₂ NCH ₂ CH ₂ - N(CH ₃) ₂	116.21	4, 250	0.770	1.4179 ²⁰	-55	120–122	10	
t109	Tetramethyl- germanium	(CH ₃) ₄ Ge	132.73		1.006^{0}	1.3871 ²⁰	-88	43.4		
t110	1,1,3,3-Tetramethyl- guanidine	$[(CH_3)_2N]_2C = NH$	115.18					163		
t111	N,N,N',N'-Tetra- methyl-1,6-hexane- diamine	[(CH ₃) ₂ N(CH ₂) ₃ —] ₂	172.32	4 ¹ , 423	0.806	1.4359 ²⁰		209–210	73	
t112	Tetramethyllead	(CH ₃) ₄ Pb	267.33	4, 639	1.995_4^{20}		-27.5	110		misc alc, eth

t113	N,N,N',N'-Tetra- methyl-	(CH ₃) ₂ NCH ₂ N(CH ₃) ₂	102.18	4, 54	0.749 ²⁰	1.4005		85	<1	
t114	methanediamine Tetramethyl ortho- carbonate	C(OCH ₃) ₄	136.15	$3^2, 4$	1.023	1.3845 ²⁰	-5	114	6	
t115	2,6,10,14-Tetra- methylpentadecane	[(CH ₃) ₂ CH(CH ₂) ₃ - CH(CH ₃)CH ₂] ₂ CH ₂	268.53		0.7827_4^{20}	1.4379^{20}	-100	167 ^{11mm}		s bz, chl, eth, PE
t116	2,3,5,6-Tetramethyl- phenol	(CH ₃) ₄ C ₆ HOH	150.22	6, 547			108–110	250		
t117	2.2,6,6-Tetramethyl- piperidino-N-oxy- (free radical)		156.25				36–38		67	
t118	N,N,N',N'-Tetra- methyl-1,3-propane- diamine	(CH ₃) ₂ N(CH ₂) ₃ N(CH ₃) ₂	130.24	4, 262		1.4234 ²⁰		145–146	31	
t119	Tetramethylpyrazine		136.20	23, 99			84-86	190		
t120 t121	Tetramethylsilane 1,2,2,3-Tetramethyl-	(CH ₃) ₄ Si [(C ₆ H ₅) ₂ Si(CH ₃)O] ₂ -	88.23 484.8	4, 625	$0.6411_4^{20} \\ 1.07_4^{20}$	$1.3585^{20} \\ 1.551^{25}$	-99.5	26.5 235 ^{0.5mm}	-27 221	v s alc, eth
	1,1,3,3-tetra- phenyltrisiloxane	Si(CH ₃) ₂								

2,2,5,5-Tetramethyl-3,4-dithiahexane, d114 Tetramethylene chlorobromide, b251 Tetramethylethylene glycol, d491 Tetramethylene oxide, t66 Tetramethylene sulfide, t81 Tetramethylolmethane, p20 2,2,4,4-Tetramethyl-3-thiapentane, d133 Tetramethylthiuram disulfide, b174

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t122	1,1,3,3-Tetramethyl-	$(CH_3)_2NC(=S)N(CH_3)_2$	132.23	4 ¹ , 336			75–77	245		
	2-thiourea									
t123	Tetramethyltin	(CH ₃) ₄ Sn	178.83	4, 631	1.3149 ²⁵	1.5201	-54.8	78		
t124	1,1,3,3-Tetramethyl-	$(CH_3)_2NC(=O)N(CH_3)_2$	116.16	4, 74	0.9687_4^{20}	1.449325	-1.2	176	65	misc aq, alc, chl,
4104-	urea Tetranitromethane	C(NO.)	106.02	1 00	1 (22025	1 42 5025	13.5	126	> 112	eth
t124a t125		$C(NO_2)_4$	196.03	1,80	1.6229 ²⁵ 1.089	1.4358^{25} 1.4621^{20}	16	126	>112	v s alc, eth, alk
1125	1,4,7,10-Tetraoxa- cyclododecane		176.21		1.089	1.4021-	10		>112	
t126	2,4,8,10-Tetraoxa-		160.17	19, 436			52-55	83 ^{1.5mm}		
	spiro[5.5]undecane									
t127	Tetraphenoxysilane	(C ₆ H ₅ O) ₄ Si	400.5		1.141_4^{60}	1.55460	48-49	237 ^{1mm}		
t128	Tetraphenylboron	$(C_6H_5)_4B^-Na^+$	342.23				>300			v s aq, acet; s chl
	sodium									
t129	1,1,4,4-Tetraphenyl-	$(C_6H_5)_2C=CHCH=C-$	358.49	5, 750			207–209			
	1,3-butadiene	$(C_6H_5)_2$			2.5					
t130	1,1,3,3-Tetraphenyl-	$[(C_6H_5)_2Si(CH_3)]_2O$	410.7		1.076_4^{25}	1.5866^{26}	50	215 ^{0.5mm}	193	
	1,3-dimethyldi-									
.121	siloxane	(GH) G G(GH)	222.45	5 542			222 224	420		
t131	Tetraphenylethylene	$(C_6H_5)_2C = C(C_6H_5)_2$	332.45	5, 743	1.0784		222–224	420 228 ^{3mm}		
t132 t133	Tetraphenylsilane Tetraphenyltin	$(C_6H_5)_4Si$ $(C_6H_5)_4Sn$	336.5 427.11		1.078_{4}° 1.490°		236–237 226	>420	110	
t133	Tetrapropoxysilane	$(C_6H_5)_4SII$ $(C_3H_7O)_4Si$	264.4		0.916_4^{20}	1.401^{20}	220	94 ^{5mm}	110	
t134	Tetrapropylam-	(CH ₃ CH ₂ CH ₂) ₄ N ⁺ Br ⁻	266.27	4 ¹ , 364	0.9104	1.401	270 d	94		s aq
1133	monium	(C113C112C112)41V B1	200.27	7,504			270 u			s aq
	bromide									
t136	1 <i>H</i> -Tetrazole		70.06	26, 346			156–158	subl		s ag, alc, acet
t137	2-Thenoyltrifluoro-		222.18	, ´			40–44	98 ^{8mm}		A: /
	acetone									
	•	•		'		'				•

t138	Theobromine		180.17	26, 457			357	subl 290		0.05 aq; 0.045 alc; s alk; i bz, chl,
										eth
t139	Thiamine HCl		337.27				d 248			100 aq; 1 alc
t140	Thiazole		85.13	27, 15	1.200^{17}	1.5375^{20}		117-118	22	s alc, eth; sl s aq
t141	Thioacetamide	$CH_3C(=S)NH_2$	75.13	2, 232			112-114			16 aq; sl s alc, eth
t142	Thioacetic acid	CH ₃ O—SH	76.12	2, 230	1.065	1.4630^{20}	<-17	88-91	< 1	s aq; misc alc, eth
t143	Thiobenzoic acid	C ₆ H ₅ CO—SH	138.19	9,419	1.174	1.6020^{20}	15-18	d	>112	misc eth; v s alc; i
										aq

Tetrantoin, b40

2,5,8,13-Tetraoxadodecane, b189

3,6,9,12-Tetraoxatridecanol, t53

Tetraphene, b6

2-Thenoic acid, t157

2-Thiabutane, e182

Thiacyclobutane, t345a

1-Thia-3-cyclopentene, 1,1-dioxide, d368

3-Thiaheptane, b451

2-Thiahexane, b463

3-Thiahexane, e210 Thianaphthene, b61 5-Thianonane, d132

2-Thiapentane, m395

3-Thiapentane, d337 Thioanisole, m364

2-Thiobarbituric acid, d388

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t138

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t144	4,4'-Thiobis(2- <i>tert</i> -butyl-6-methyl-phenol)		358.54				127	316 ^{40mm}	240	
t145	4,4'-Thiobis(1,3-dihydroxybenzene)	$[(HO)_2C_6H_3]_2S$	250.27	6 ³ , 6291			175–177			
t146	Thiocarbanilide	C ₆ H ₅ NHCSNHC ₆ H ₅	228.32	12, 394	1.32^{24}		154			v s alc, eth
t147	p-Thiocresol	HSC ₆ H ₄ CH ₃	124.21	6, 416			43-44	195	68	s alc, eth; i aq
t148	2,2'-Thiodiacetic acid	(HOOCCH ₂) ₂ S	150.15	3, 253			129			s aq, alc
t149	2,2'-Thiodiethanol	(HOCH ₂ CH ₂) ₂ S	122.19	1,470	1.1824_4^{20}	1.5203 ²⁰	-16	282	110	misc aq, alc; sl s eth
t150	4,4'-Thiodiphenol	(HOC ₆ H ₄) ₂ S	218.27	6,860			150-155			
t151	3,3'-Thiodipropionic acid	(HOOCCH ₂ CH ₂) ₂ S	178.21				134			3.4 aq; v s alc
t152	2-Thiohydantoin		116.14	24, 260			231 d			sl s aq; i alc, eth
t153	N-Thionylaniline	$C_6H_5N=SO$	139.18	12, 578	1.236	1.6270^{20}		200		_
t154	Thiophene	C_4H_4S	84.14	17, 29	1.0573_4^{25}	1.5257 ²⁵	-38.2	84.2	-1	misc alc, eth; i aq
t155	2-Thiopheneacetic acid	(C ₄ H ₃ S)CH ₂ COOH	142.18	18, 293			63–67	160 ^{22mm}		_
t156	2-Thiophenecarb- aldehyde	(C ₄ H ₃ S)CHO	112.15	17, 285	1.200	1.5900 ²⁰		198	77	s eth
t157	2-Thiophenecarb- oxylic acid	(C ₄ H ₃ S)COOH	128.15	18, 289			128.5	260		s aq, chl; v s alc, eth
t158	2-Thiophenemethyl- amine	(C ₄ H ₃ S)CH ₂ NH ₂	113.19	18 ⁴ , 7096	1.103	1.5569 ²⁰		99 ^{28mm}	73	
t159	Thiophenol	C ₆ H ₅ SH	110.18	6, 294	1.0766 ²⁰	1.5897 ²⁰	-14.9	169.1	50	v s alc; misc bz, eth
t160	Thiophenoxyacetic acid	C ₆ H ₅ SCH ₂ COOH	168.21	6, 313			64–66			

t161	Thiopropionic acid	CH ₃ CH ₂ CO—SH	90.14	2, 264	1.014	1.4640^{20}		108-110	11	
t162	3-Thiosemicarbazide	$H_2NC(=S)NHNH_2$	91.14	3, 195			182 - 184			s aq, alc
t163	Thiourea	$H_2NC(=S)NH_2$	76.12	3, 180	1.045		176-178			9 aq; s alc; sl s eth
t164	1,4-Thioxane		104.17	19, 3	1.114	1.5095^{20}		147	42	
t165	Thioxanthen-9-one		212.27	17, 357			211	273 ^{715mm}		v s bz, chl, hot
										HOAc
t166	Titanium(IV) iso-	Ti[OCH(CH ₃) ₂] ₄	284.26	1 ² , 382	0.955	1.4654^{20}	18-20	218 ^{10mm}	22	
	propoxide	37231								
t167	Toluene	C ₆ H ₅ CH ₃	92.14	5, 280	0.8660_4^{20}	1.4969^{20}	-95.0	110.6	7	misc alc, chl, eth,
										acet, HOAc
t168	2,4-Toluenediamine	CH ₃ C ₆ H ₃ (NH ₂) ₂	122.17	13, 124			97-99	283.5		s hot aq, alc, eth
t169	2,5-Toluenediamine	$CH_3C_6H_3(NH_2)_2$	122.17	13, 144			64	273-274		v s aq, alc, eth
t170	2,6-Toluenediamine	CH ₃ C ₆ H ₃ (NH ₂) ₂	122.17	13, 148			104-106			s ag, alc
t170 t171	2,6-Toluenediamine 3,4-Toluenediamine	CH ₃ C ₆ H ₃ (NH ₂) ₂ CH ₃ C ₆ H ₃ (NH ₂) ₂	122.17 122.17	13, 148 13, 148				156 ^{18mm}		s aq, alc v s aq
	*	3 0 31 2/2		l *	1.2244 ²⁰	1.5689 ²⁰		156 ^{18mm} 251	121	v s aq
t171	3,4-Toluenediamine	$CH_3C_6H_3(NH_2)_2$	122.17	13, 148	1.2244 ²⁰	1.5689 ²⁰	88-90		121	1.

Thiocarbanilide, d692 2,2'-Thiodiethanethiol, b187 Thiodiethylene glycol, t149 Thiodiglycol, t149 Thiodiglycolic acid, t148 Thioethanolamine, a162 1-Thioglycerol, m20 Thioglycolic acid, m14 Thiolactic acid, m21 Thiomalic acid, m23 4,4'-Thioresorcinol, t145 Thiosalicyclic acid, m16 Thiosinamine, a101 2-Thixo-4-thiazolidinone, r3 Threonine, a187 Tiglic acid, m161 Tioxolone, h104 TMS, t120 TMSDEA, t371 TMSI, t373 Tolazoline, b102 p-Tolualdehyde, m126 Toluenethiols, p128, t147

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TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t173	p-Toluenesulfinic acid	CH ₃ C ₆ H ₄ SO ₂ H	172.20	11,9			85			v s alc, eth
t174 t175	p-Toluenesulfonamide p-Toluenesulfonyl- hydrazide	CH ₃ C ₆ H ₄ SO ₂ NH ₂ CH ₃ C ₆ H ₄ SO ₂ NHNH ₂	171.22 186.23	11, 104 11 ² , 66			137–140 110 d			0.2 aq; 3.6 alc
t176	<i>p</i> -Toluenesulfonic acid	CH ₃ C ₆ H ₄ SO ₃ H	172.20	11,97				140 ^{20mm}		67 aq; s alc, eth
t177	<i>p</i> -Toluenesulfonyl chloride	CH ₃ C ₆ H ₄ SO ₂ Cl	190.65	11, 103			69–71	134 ^{10mm}		v s alc, bz, eth; i aq
t178	<i>p</i> -Toluenesulfonyl fluoride	CH ₃ C ₆ H ₄ SO ₂ F	174.19	11 ² , 54			41–42	112 ^{16mm}		
t179	<i>p</i> -Toluenesulfonyl isocyanate	CH ₃ C ₆ H ₄ SO ₂ NCO	197.21			1.4355^{20}		144 ^{10mm}		
t180	o-Toluidine	CH ₃ C ₆ H ₄ NH ₂	107.16	12,772	0.9984^{20}	1.5725^{20}	-16.1	200.4	85	1.7 aq; s alc, eth
t181	<i>m</i> -Toluidine	CH ₃ C ₆ H ₄ NH ₂	107.16	12, 853	0.989_4^{20}	1.5681^{20}	-30.4	203.4	85	misc alc, eth
t182	<i>p</i> -Toluidine	CH ₃ C ₆ H ₄ NH ₂	107.16	12,880	1.046_4^{20}	1.5532^{59}	43.8	200.6	88	7.4 aq; v s alc, eth
t183	1-(<i>o</i> -Toluidino)-1,3- butanedione	CH ₃ C ₆ H ₄ NHCOCH ₂ - COCH ₃	191.23	12, 823			104–106	143		-
t184	o-Tolunitrile	CH ₃ C ₆ H ₄ CN	117.15	9, 466	0.9955_4^{20}	1.5279^{20}	-13	205.2	84	i aq; misc alc, eth
t185	<i>m</i> -Tolunitrile	CH ₃ C ₆ H ₄ CN	117.15	9, 477	0.976^{15}	1.5256^{20}	-23	210	86	0.09 aq; v s alc, eth
t186	<i>p</i> -Tolunitrile	CH ₃ C ₆ H ₄ CN	117.15	9, 489	0.9785_4^{30}		29.5	217.6		i aq; v s alc, eth
t187	o-Toluoyl chloride	CH ₃ C ₆ H ₄ COCl	154.60	9, 464	1.185	1.5549^{20}		90 ^{12mm}	76	
t188	m-Toluoyl chloride	CH ₃ C ₆ H ₄ COCl	154.60	9, 477	1.173	1.5485^{20}		86 ^{5mm}	76	
t189	p-Toluoyl chloride	CH ₃ C ₆ H ₄ COCl	154.60	9, 484	1.169	1.5535^{20}	-2	225–257	82	
t190	m-Tolyl isocyanate	CH ₃ C ₆ H ₄ NCO	133.15	12, 864	1.033	1.5305^{20}		76 ^{12mm}	65	s alc, eth; i aq
t191	(p-Tolylsulfonyl)-	CH ₃ C ₆ H ₄ SO ₂ CH ₂ NC	195.24				114–115			
	methyl isocyanide									
t192	<i>p</i> -Tolyltrichlorosilane	CH ₃ C ₆ H ₄ SiCl ₃	225.6		1.3420			218–220		

t193	1,2,4-Triacetoxy-	C ₆ H ₃ (OOCCH ₃) ₃	252.22	6, 1089			98-100			
	benzene									
t194	Triacetoxyethyl-	$C_2H_5Si(OOCCH_3)_3$	234.3		1.1428_4^{20}	1.4123^{20}		107-		
	silane							108 ^{8mm}		
t195	Triacetoxyvinyl-	(CH ₃ COO) ₃ SiCH=CH ₂	232.3		1.167_4^{20}	1.423^{20}		113 ^{1mm}	104	
	silane									
t196	1,3,5-Triacetyl-	$C_6H_3(COCH_3)_3$	204.23	7,866			160-162		17	
	benzene									
t197	Triallyl-s-triazine-		249.27			1.5129^{20}		152 ^{4mm}	>112	
	2,4,6(1H,3H,5H)-									
	trione									
t198	2,4,6-Triamino-		126.12	26, 245	1.573^{250}		>250	subl		sl s aq; i alc, eth
	1,3,5-triazine									_
t199	1H-1,2,4-Triazole		69.07	26, 13			119-121	260 d		s aq, alc
t200	Tribenzylamine	(C ₆ H ₅ CH ₂) ₃ N	287.41	12, 1038	0.991_4^{95}		91-94		65	s hot alc, eth
t201	Tribromoacetaldehyde	Br ₃ CCHO	280.76	1,626	2.665	1.5850^{20}		174	65	s aq, alc, chl, eth
t202	Tribromoacetic acid	Br ₃ CCOOH	296.76	2, 220			130-133	245 d		s aq, alc, eth
t203	2,4,6-Tribromoaniline	Br ₃ C ₆ H ₂ NH ₂	329.83	12,663	2.35		120-122	300		s hot alc, chl, eth
t204	2,2,2-Tribromoethanol	Br ₃ CCH ₂ OH	282.77	1 ² , 338			80-81	93 ^{10mm}		2 aq; s alc, bz, eth
t205	1,1,2-Tribromo-	BrCH=CBr ₂	264.74	1, 191	1.708^{21}	1.6247^{25}		162.5		_
	ethylene									

Toluic acids, m130, m131, m132 α -Tolunitrile, p80

p-Tolylacetamide, m355 Triacetin, p201 1,3,5-Triazine-2,4,6-triol, c299 Tributyl borate, t209

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t206	Tribromomethane	CHBr ₃	252.77	1, 68	2.903115	1.600515	8.1	149.6	none	0.3 aq; misc eth,
t207	2,4,6-Tribromophenol	Br ₃ C ₆ H ₂ OH	330.82	6, 203	2.55		94–96	244		MeOH s alc, chl, eth; i aq
t208	1,2,3-Tribromo-	BrCH ₂ CH(Br)CH ₂ Br	280.78	1, 112	2.411415		16–17	219–221		s alc, eth
	propane									
t209	Tributoxyborane	$(C_4H_9O)_3B$	230.16	$1^2,398$	0.8580^{20}	1.409220	-70	233.5	93	hyd aq
t210	Tributylamine	$(C_4H_9)_3N$	185.36	4, 157	0.7784_4^{20}	1.428320	-70	216–217	63	v s alc, eth; s acet
t211	2,4,6-Tri- <i>tert</i> -butylphenol	[(CH ₃) ₃ C] ₃ C ₆ H ₂ OH	262.44		0.864_4^{27}		131	278		
t212	Tributyl phosphate	$(C_4H_9O)_3P(O)$	266.32	1 ² , 397	0.972^{25}	1.422625	<-80	289 d	146	0.04 aq; misc org
										solv
t213	Tributylphosphine	$(C_4H_9)_3P$	202.32	$4^2,971$	0.812	1.4619^{20}		150 ^{50 mm}	40	
t214	Tributyl phosphite	$(C_4H_9O)_3P$	250.32	1 ¹ , 187	0.925_4^{20}	1.4326 ²⁰		125 ^{7mm}	121	misc alc, bz, eth, PE
t215	Tributyltin chloride	$(C_4H_9)_3$ SnCl	325.49		1.200	1.490520		173 ^{25mm}	>112	I L
t216	Trichloroacetic acid	Cl ₃ CCOOH	163.39	2, 206	1.629_4^{61}		57–58	196-197		120 aq; v s alc, eth
t217	Trichloroaceto-	Cl ₃ CCN	144.39	2, 212	1.440345	1.4409^{20}		85.7	none	
	nitrile									
t218	Trichloroacetyl chloride	Cl ₃ CCOCl	181.83	2, 210	1.629	1.4689 ²⁰		114–116	none	
t219	Trichloroacetyl	Cl ₃ CC(=O)NCO	188.40			1.480920		85 ^{20mm}	65	
	isocyanate									
t220	2,4,5-Trichloro- aniline	Cl ₃ C ₆ H ₂ NH ₂	196.46	12, 627			93–95	270		s alc
t221	2,4,6-Trichloro-	Cl ₃ C ₆ H ₂ NH ₂	196.46	12,627			73–75	262		s alc, eth
	aniline	3 0 2 2								,
t222	1,2,3-Trichloro-	C ₆ H ₃ Cl ₃	181.45	5, 203	1.69_{25}^{25}		52.6	221	113	v s bz, CS ₂
	benzene									
t223	1,2,4-Trichloro-	C ₆ H ₃ Cl ₃	181.45	5, 204	1.446 ²⁵	1.5707 ²⁰	17	214	110	misc bz, eth, PE
	benzene									

t224	1,3,5-Trichloro-	C ₆ H ₃ Cl ₃	181.45	5, 204		1.566219	63.4	208.5	107	v s bz, eth, PE
t225	benzene 2,2,2-Trichloro-1,1- dimethylethyl chloroformate	CICOOC(CH ₃) ₂ CCl ₃	239.92				30–32	83- 84 ^{14mm}	none	
t226	1,1,1-Trichloro- ethane	CH ₃ CCl ₃	133.41	1,85	1.3376420	1.4379^{20}	-30.4	74.0	none	0.13 aq; s bz, eth
t227	1,1,2-Trichloro- ethane	CICH ₂ CHCl ₂	133.41	1, 85	1.4416 ²⁰	1.4711 ²⁰	-36.6	113.5	none	0.4 aq; misc alc, eth
t228	2,2,2-Trichloro- ethanol	Cl ₃ CCH ₂ OH	149.40	1, 338	1.557_{20}^{20}	1.4885^{20}	17.8	151		8 aq; misc alc, eth
t229	2,2,2-Trichloro- ethyl chloroformate	CICOOCH ₂ CCl ₃	211.86		1.539	1.4703^{20}		171–172	none	
t230	1,1,2-Trichloro- ethylene	CICH=CCl ₂	131.39	1, 187	1.4649420	1.4775^{20}	-84.8	86.7	none	0.1 aq; misc alc, chl, eth
t231 t232	Trichloroethylsilane Trichlorofluoro-	C ₂ H ₅ SiCl ₃ Cl ₃ CF	163.5 137.4		$\begin{vmatrix} 1.2373_4^{20} \\ 1.485^{21} \end{vmatrix}$	$1.4256^{20} \\ 1.384^{20}$	-106 -111	100.5 23.8	27	0.14 aq; s alc, eth
t233	methane $\alpha, \alpha, 2$ -Trichloro-6-fluorotoluene	ClC ₆ H ₃ (F)CHCl ₂	213.47	5 ³ , 701	1.446	1.5506 ²⁰		228–230	>112	
t234	Trichloroisocyanuric acid		232.41	25, 256			249–251			

Tributyrin, g19 β , β , β -Trichloroethoxycarbonyl chloride, t229

Trichloromethane, c126 Trichlorophenylsilane, p155 3,3,3-Trichloropropylene oxide, e13

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t235	Trichloromethane- sulfenyl chloride	Cl ₃ CSCl	185.89	3, 135	1.700_4^{20}	1.5436 ²⁰		146–148	none	
t236	Trichloromethane sulfonyl chloride	Cl ₃ CSO ₂ Cl	217.88	3 ² , 16			139			s alc, eth
t237	1,1,1-Trichloro-2- methyl-2-propanol	(CH ₃) ₂ C(OH)CCl ₃	177.46	1, 382			99	167		s alc, bz, chl, eth
t238	Trichloromethyl- silane	CH ₃ SiCl ₃	149.48		1.275_4^{20}	1.410820	-90	66	5	
t238a	1,2,4-Trichloro-5-	Cl ₃ C ₆ H ₂ NO ₂	226.45	5, 246	1.790^{20}		49–55	288		v s bz, eth
t239	Trichloronitro- methane	Cl ₃ CNO ₂	164.38	1,76	1.6558 ²⁰	1.4611 ²⁰	-64	112		misc alc, bz; s eth
t240	2,4,5-Trichloro- phenol	Cl ₃ C ₆ H ₂ OH	197.45	6 ² , 180			67	253		615 acet; 163 bz; 525 eth; s alc; i
t241	2,4,6-Trichloro- phenol	Cl ₃ C ₆ H ₂ OH	197.45	6, 190	1.4901 ⁷⁵		69	246	none	525 acet; 113 bz; 354 eth; v s alc; i aq
t242	(2,4,5-Trichloro- phenoxy)acetic acid	Cl ₃ C ₆ H ₂ OCH ₂ COOH	255.49	6 ³ , 702			153			s alc; v sl s aq
t243	2-(2,4,5-Trichloro- phenoxypropionic	Cl ₃ C ₆ H ₂ O- CH(CH ₃)COOH	269.51				181.6			0.14 aq; 16 acet; 0.16 bz; 7.1 eth
t244	1,2,3-Trichloro- propane	ClCH ₂ CH(Cl)CH ₂ Cl	147.43	1, 106	1.3880 ²⁰	1.4834 ²⁰	-14.7	156.9	82	misc alc, eth; i aq
t245	1,1,1-Trichloro-2- propanol	CH ₃ CH(OH)CCl ₃	163.43	1,365			50	162	82	2.9 aq; v s alc, eth

t246	2,4,6-Trichloro-		183.43	23, 90		1.5700^{20}	23–25	210–215	>112	
	pyrimidine									
t247	Trichlorosilane	HSiCl ₃	135.45		1.3417_4^{20}	1.400^{20}	-1.28	31–32	-20	d aq; s bz, chl
t248	α, α, α -	C ₆ H ₅ CCl ₃	195.48	5,300	1.3756_4^{20}	1.5570^{20}	-5.0	220.8	97	s alc, bz, eth
	Trichlorotoluene									
t249	α ,2,6-Trichloro-	Cl ₂ C ₆ H ₃ CH ₂ Cl	195.48				36-39	119 ^{14mm}		v s alc, eth
	toluene									
t250	2,4,6-Trichloro-		184.41	26, 35			148	190 ^{720mm}		i aq; s alc
	1,3,5-triazine									_
t251	1,1,2-Trichloro-	Cl ₂ CFCClF ₂	187.38	$1^3, 157$	1.563525	1.3557^{25}	-36.4	47.6	none	0.017 aq
	trifluoroethane			,						,
t252	Trichlorovinyl-	H ₂ C=CHSiCl ₂	161.49		1.24320	1.4300^{20}	-95	90-93	-9	
	silane	2 3			-					
t253	Tricyclo[5.2.1.0 ^{2,6}]-		136.24	5, 164			77–79	193	40	
	decane			-,						
t254	Tricyclo[5.2.1.0 ^{2,6}]-		150.22	7^2 , 133	1.063	1.5025^{20}		132 ^{30mm}		
1231	decan-8-one		130.22	, , 133	1.003	1.5025		132		
t255	1,3,5-Tricyclohexyl-		333.57				74–75	97 ^{6mm}		
(233	hexahydro-s-		333.37				74 73			
	triazine		I	I	1	l	1	1	l	

Tricine, t428

Tricyclo[3.3.1.1^{3,7}]decane, a67

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t256 t257 t258 t259	Tridecane Tridecanoic acid 1-Tridecene Triethanolamine	CH ₃ (CH ₂) ₁₁ CH ₃ CH ₃ (CH ₂) ₁₁ COOH CH ₃ (CH ₂) ₁₀ CH=CH ₂ (HOCH ₂ CH ₂) ₃ N	184.37 214.35 182.35 149.19	1, 171 2, 364 1, 225 4, 285	$0.7563_4^{20} 0.7653_4^{20} 1.1242_4^{20}$	1.4256 ²⁰ 1.4334 ²⁰ 1.4835 ²⁵	-5.4 41-42 -23.1 21.6	235.4 236 ^{100mm} 232.8 335.4	79 79 185	v s alc, eth v s alc, eth; i aq s alc; v s eth misc aq, alc, acet; 4.5 bz; 1.6 eth; s chl
t260 t261	Triethoxyborane Triethoxyethyl- silane	(CH ₃ CH ₂ O) ₃ B (C ₂ H ₅ O) ₃ SiC ₂ H ₅	145.99 192.3	1, 335	$0.864_{20}^{20} \\ 0.8963_4^{20}$	$ \begin{array}{c} 1.3740^{20} \\ 1.3955^{20} \end{array} $		117–118 158–159	11	d aq
t261a	Triethoxymethyl-silane	$CH_3Si(OC_2H_5)_3$	178.30	4, 629	0.895_4^{20}	1.3845 ²⁰		141–143	23	s alc
t261b t262	Triethoxysilane Triethoxyvinyl- silane	$(C_2H_5O)_3SiH$ $(C_2H_5O)_3SiCH=CH_2$	164.28 190.32	1,334	$0.875_4^{20} \\ 0.903_4^{20}$	1.3762 1.3978 ²⁰		131.5 160–161	26 34	
t263	Triethylaluminum	$(C_2H_5)_3Al$	114.17	4, 643	0.832^{25}		-58	194		d aq, air
t264	Triethylamine	$(C_2H_5)_3N$	101.19	4,99	0.7326 ₄ ²⁵	1.3980 ²⁵	-114.7	89.6	-6	5.5 aq; misc alc, eth; s acet, EtAc
t265 t266 t267	Triethylantimony Triethylarsine Triethylbismuthine	$(C_2H_5)_3Sb$ $(C_2H_5)_3As$ $(C_2H_5)_3Bi$	208.94 162.11 296.17	4, 618 4, 602 4, 622	$ \begin{array}{c} 1.324^{16} \\ 1.150_4^{20} \\ 1.82 \end{array} $	1.42	-29	159.5 140 ^{736mm} 107 ^{79mm}		i aq; misc alc, eth i aq; v s alc, eth
							explodes v	when heated	in air	-
t268 t269	Triethylborane Triethylenediamine	$(C_2H_5)_3B$	98.00 112.18	4, 641	0.6961 ²³		-92.9 158	95 174		i aq; d air 45 aq; 13 acet; 77 alc; 51 bz
t270 t271	Triethylene glycol Triethylene glycol dibenzoate	(HOCH ₂ CH ₂ OCH ₂ —) ₂ (C ₆ H ₅ COOCH ₂ - CH ₂ OCH ₂ —) ₂	150.17 358.39	1,468	$ \begin{array}{c} 1.1274_4^{15} \\ 1.2715^{30} \end{array} $	1.4578 ¹⁵ 1.5252 ⁵⁰	-4.3 47	285	165	misc aq, alc, bz
t272	Triethylenetetramine	$(H_2NCH_2CH_2NHCH_2-)_2$	146.24	4, 255	0.982	1.4971^{20}	12	266–267	143	

t273	<i>N,N,N'</i> -Triethyl-ethylenediamine	(C ₂ H ₅) ₂ NCH ₂ CH ₂ - NHC ₂ H ₅	144.26	4^2 , 691	0.804	1.4311^{20}		55 ^{13mm}	32	
t274	Triethylgallium	$(C_2H_5)_3Ga$	156.91		1.0576^{30}		-82.3	142.6		
t275	1,3,5-Triethylhexa-		171.29	26, 2	0.894	1.4595^{20}		207-208		
	hydro-s-triazine									
t276	Triethylindium	$(C_2H_5)_3In$	202.01		1.260^{20}	1.538^{20}	-32	144		
t277	Triethyl ortho- acetate	$CH_3C(OC_2H_5)_3$	162.23	2, 129	0.8847_4^{25}	1.3950^{25}		142	55	misc alc, chl, eth
t278	Triethyl ortho-	HC(OC ₂ H ₅) ₃	148.20	2, 20	0.891_4^{20}	1.3919^{20}	-76	146	30	d aq; s alc, eth
	formate									
t279	Triethyl ortho-	$CH_3CH_2C(OC_2H_5)_3$	176.26	2, 240	0.876	1.3995^{20}		155-160	60	v s alc, eth
	propionate									
t280	Triethyl phosphate	$(C_2H_5O)_3P(O)$	182.16	1,332	1.0725^{19}	1.4045^{20}		215–216		s aq(d), alc, eth
t281	Triethylphosphine	$(C_2H_5)_3P$	118.16	4, 582	0.800_4^{15}		-88	129	pyro-	i aq; misc alc, eth
									phoric	
t282	Triethyl phosphite	$(C_2H_5O)_3P$	166.2	1,330	0.969_4^{20}	1.4131^{20}		65 ^{24mm}	55	i aq(hyd); misc
										alc, acet, bz,
										eth, PE
t283	Triethyl phosphono-	$(CH_3CH_2O)_2P(O)$ -	224.19	4 ¹ , 573	1.130	1.4310^{20}		145 ^{9mm}	>112	
	acetate	CH ₂ COOC ₂ H ₅								

Tridecylbenzene, p156 3-Triethoxysilylpropylamine, a279 Triethyl borate, t260 Triethylenediamine, d45 Triethylene glycol, e127 Triethylene glycol dimethyl ether, b189 O,O,O-Triethyl phosphorothioate, t285

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t284 t285	Triethylsilane Triethyl thio- phosphate	(C ₂ H ₅) ₃ SiH (C ₂ H ₅ O) ₃ P(S)	116.28 198.22	4, 625 1, 333	0.731 ₄ ²⁰ 1.082	$1.412^{20} \\ 1.4480^{20}$		107–108 100 ^{16mm}	107	i aq; misc alc, eth
t286	2,2,2-Trifluoro- acetamide	CF ₃ CONH ₂	113.04	2^2 , 186			75	162.5		
t287 t288	Trifluoroacetic acid Trifluoroacetic anhydride	CF ₃ COOH [CF ₃ C(O)] ₂ O	114.02 210.03	2 ² , 186 2 ² , 186	1.4890 ²⁰ 1.487	$1.2850^{20} > 1.30$	-15.3 -65	71.8		misc aq
t289	α,α,α -Trifluoro- acetophenone	C ₆ H ₅ COCF ₃	174.12		1.240	1.4595^{20}		165–166	41	
t290	α, α, α -Trifluoro- m-cresol	CF ₃ C ₆ H ₄ OH	162.11	6 ¹ , 187	1.333	1.4588 ²⁰	-1.8	178–179	73	
t291 t292	1,1,1-Trifluoroethane 2,2,2-Trifluoro- ethanol	CH ₃ CF ₃ CF ₃ CH ₂ OH	84.04 100.04		1.3842420	1.2907 ²²	-111.3 -43.5	-47.3 74.1	29	
t293	2,2,2-Trifluoro- ethyl acrylate	CF ₃ CH ₂ OOCCH=CH ₂	154.0		2.142_4^{25}	1.3981 ²⁵		46 ^{125mm}		
t294	2,2,2-Trifluoro- ethyl trifluoro- acetate	CF ₃ CH ₂ OOCCF ₃	196.0		1.4725 ₄ ¹⁸	1.281218	-65.5	55		
t295	Trifluoromethane	HCF ₃	70.01	1,59	1.52^{-100}		-155.2	-82.2		75 mL aq; 500 mL alc
t296	Trifluoromethane- sulfonic acid	CF ₃ SO ₃ H	150.07	$3^3, 34$	1.695 ²⁵	1.3250^{25}	34	162	none	v s aq; misc eth
t297	Trifluoromethane- sulfonic anhydride	(CF ₃ SO ₂) ₂ O	282.13	3 ⁴ , 35	1.677	1.3212^{20}		84		d aq, alc
t298	3-(Trifluoromethyl)- benzonitrile	CF ₃ C ₆ H ₄ CN	171.12	9, 478	1.2813 ²⁰	1.4505 ²⁰	14.5	189	72	

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$											
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	t299		CF ₃ C ₆ H ₄ CH ₂ Cl	194.59		1.254	1.4605		70 ^{12mm}		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	t300	α,α,α -Trifluoro-	C ₆ H ₅ CF ₃	146.11	5, 290	1.1886 ²⁰	1.4145^{20}	-29	102	12	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Trihexylamine	2 3 2 2 3 2 3		4, 188	0.07120	1 45 620			>112	v s alc, eth; i aq
t304 1,2,3-Trihydroxy-benzene 1,3,5-Trihydroxy-benzene 1,3,5-Trihydroxy-benzene 1305 1,3,5-Trihydroxy-benzene 1306 3,4,5-Trihydroxy-benzene 1307 Triisodecyl phosphite 1308 Triisodecyl phosphite 1310 Triisopropoxyborane 1311 Triisopropoxyborane 1311 Triisopropoxyinyl-silane 1312 1,3,5-Triisopropyl-benzene 1313 Triisopropyl-benzene 1314 Triisopropyl-benzene 1315 Triisopropyl-benzene 1316 Triisopropyl-benzene 1316 Triisopropyl-benzene 1316 Triisopropyl-benzene 1317 Triisopropyl-benzene 1318 Triisopro	1302		[CH ₃ (CH ₂) ₅] ₃ SiCi	319.1		0.8/14	1.430-				
benzene 1,3,5-Trihydroxy-benzene 1305 1,3,5-Trihydroxy-benzene 1306 3,4,5-Trihydroxy-benzene 1307 Triisobutylaluminum [(CH ₃) ₂ CHCH ₂] ₃ Al 198.33 0.781 ²⁵ 6 86 ^{10mm} pyro-phoric 1308 Triisopropanolamine 1310 Triisopropoxyborane 1311 Triisopropoxylorane 1312 1,3,5-Triisopropyl-benzene 1313 Triisopropyl 1313 Triisopropyl 1315 Triisopropyl 1316 1308 1309 1	t303	Trihexylsilane	[CH ₃ (CH ₂) ₅] ₃ SiH	284.60			1.448^{20}		160 ^{5mm}		
benzene 3,4,5-Trihydroxy- benzoic acid (HO) ₃ C ₆ H ₂ COOH 170.12 10,470 d 235 d 235 l 1.1 aq; 17 alc; 1 eth; 20 acet; i bz, chl, PE 1307 Triisodecyl phosphite 1309 Triisopropanolamine 1310 Triisopropoxyborane 1311 Triisopropoxyvinyl- silane 1312 1,3,5-Triisopropyl 1313 Triisopropyl [(CH ₃) ₂ CH(CH ₃) ₂] ₃ C ₆ H ₃ [CH(CH ₃) ₂] ₃ 204.36 170.12 10,470 10,470 10,470 10,470 0.781 ²⁵ 0.886 ²⁵ 1.454 ²⁵ 0.886 ²⁵ 1.454 ²⁵ 0.9996 ⁵⁰ 0.886 ²⁵ 1.454 ²⁵ 0.9996 ⁵⁰ 0.8996 ⁵⁰ 0.863 ²⁵ 1.3764 ²⁰ 1.399-141 17 179-181 179-181 1313 Triisopropyl 1313 Triisopropyl 1315 1315 1316 1316 1317 1317 1317 1318 1	t304		$C_6H_3(OH)_3$	126.11	6, 1071	1.45		131–133			A
benzoic acid benzoic acid	t305		$C_6H_3(OH)_3$	126.11	6, 1092			218–220	subl d		1 aq; 10 alc; s eth
t307 Triisobutylaluminum [(CH ₃) ₂ CHCH ₂] ₃ Al 198.33 0.781 ²⁵ 6 86 ^{10mm} pyrophoric t308 Triisodecyl phosphite [(CH ₃) ₂ CH(CH ₂) ₇ O] ₃ P 502.80 0.886 ²⁵ ₁₅ 1.454 ²⁵ 0 180 ^{0.1mm} 235 t309 Triisopropanolamine [CH ₃ CH(OH)CH ₂] ₃ N 191.27 0.9996 ⁵⁰ ₂₀ 46 305.4 152 v s aq t310 Triisopropoxyborane [(CH ₃) ₂ CHO] ₃ B 188.08 1,363 0.815 1.3764 ²⁰ 0.863 ²⁵ ₄₅ 1.396 ²⁵ 1.396 ²⁵ 179–181 t311 Triisopropyl- characteristic CH=CH ₃ C ₆ H ₃ [CH(CH ₃) ₂] ₃ 204.36 5,458 0.845 1.4884 ²⁰ 232–236 86 t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P 208.24 1,363 0.914 ²⁰ ₄ 1.4101 ²⁰ 64 ^{11mm} 73 i aq (sl hyd)	t306		(HO) ₃ C ₆ H ₂ COOH	170.12	10, 470			d 235			eth; 20 acet; i
t309 Triisopropanolamine [CH ₃ CH(OH)CH ₂] ₃ N 191.27 1,363 0.815 1.3764 ²⁰ 139–141 17 179–181 179–181 1312 1,3,5-Triisopropyl- benzene t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P 208.24 1,363 0.914 ²⁰ 1.4101 ²⁰ 64 ^{11mm} 73 i aq (sl hyd)	t307	Triisobutylaluminum	[(CH ₃) ₂ CHCH ₂] ₃ Al	198.33		0.781 ²⁵		6	86 ^{10mm}	1.0	,
t309 Triisopropanolamine t310 Triisopropayborane t311 Triisopropoxyborane t311 Triisopropoxyborane t312 1,3,5-Triisopropyl- benzene t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P	t308	1	[(CH ₃) ₂ CH(CH ₂) ₇ O] ₃ P	502.80		0.886_{15}^{25}	1.454 ²⁵	< 0	180 ^{0.1mm}	235	
t310 Triisopropoxyborane t311 Triisopropoxyborane t311 Triisopropoxyvinyl- silane t312 1,3,5-Triisopropyl- benzene t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P 208.24 1,363 0.815 0.863 ²⁵ 1.3764 ²⁰ 0.863 ²⁵ 1.396 ²⁵ 179–181 17 204.36 5,458 0.845 1.4884 ²⁰ 232–236 86 t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P 208.24 1,363 0.914 ²⁰ 1.4101 ²⁰ 64 ^{11mm} 73 i aq (sl hyd)	t309	1 1	ICH,CH(OH)CH,1,N	191.27		0.9996^{50}_{20}		46	305.4	152	v s aq
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			- 3		1, 363	20	1.3764^{20}		139–141		1
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		1 1 2	2. 3.2 33		-,						
benzene t313 Triisopropyl [(CH ₃) ₂ CHO] ₃ P 208.24 1, 363 0.914 ²⁰ 1.4101 ²⁰ 64 ^{11mm} 73 i aq (sl hyd)		silane	CH=CH ₃								
t313 Triisopropyl $[(CH_3)_2CHO]_3P$ 208.24 $1,363$ 0.914_4^{20} 1.4101^{20} 64^{11mm} 73 $i \text{ aq (sl hyd)}$	t312	1,3,5-Triisopropyl-	$C_6H_3[CH(CH_3)_2]_3$	204.36	5, 458	0.845	1.4884^{20}		232-236	86	
		benzene									
	t313	1 10	[(CH ₃) ₂ CHO] ₃ P	208.24	1, 363	0.914_4^{20}	1.4101^{20}		64 ^{11mm}	73	i aq (sl hyd)

2,2,2-Trifluoroethyl mesylate, m438 2-(Trifluoromethyl)aniline, a129 3-(Trifluoromethyl)aniline, a130 *m*-Trifluoromethylphenol, t290 4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione, t137 α , α , α -Trifluorotoludines, a129, a130, a131 α , α , α -Trifluorotolunitrile, t298

Triglyme, b189 Tri-(2-hydroxyethyl)amine, t259 1,2,6-Trihydroxyhexane, h65 Triiodomethane, i36

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t314	3,4,5-Trimethoxy- benzaldehyde	(CH ₃ O) ₃ C ₆ H ₂ CHO	196.20	8, 391			73–75	165 ^{10mm}		
t315	1,2,3-Trimethoxy- benzene	$C_6H_3(OCH_3)_3$	168.19	6, 1081	1.112		43–45	241		
t316	3,4,5-Trimethoxy- benzoic acid	(CH ₃ O) ₃ C ₆ H ₂ COOH	212.20	10, 481			168–171	227 ^{10mm}		v s alc, eth; s chl
t317	3,4,5-Trimethoxy- benzoyl chloride	(CH ₃ O) ₃ C ₆ H ₂ COCl	230.65	10, 487			79–81	185 ^{18mm}		
t318	3,4,5-Trimethoxy- benzyl alcohol	(CH ₃ O) ₃ C ₆ H ₂ CH ₂ OH	198.22	6, 1159	1.233	1.5459 ²⁰		228 ^{25mm}	>112	
t319	Trimethoxyborane	(CH ₃ O) ₃ B	103.91	1, 287	0.920_4^{23}	1.3568 ²⁰	-34	67–68	-1	hyd aq; misc alc, eth
t320	Trimethoxyboroxine	$[-OB(OCH_3)-]_3$	173.53		1.195	1.3996 ²⁰	10	130	10	
t321	1,3,3-Trimethoxy- butane	(CH ₃ O) ₂ C(CH ₃)CH ₂ - CH ₂ OCH ₃	148.20	1 ³ , 3214	0.940	1.4096 ²⁰		63 ^{20mm}	45	
t321a	Trimethoxy(methyl)- silane	CH ₃ Si(OCH ₃) ₃	136.23		0.9548_4^{20}	1.3696 ²⁰		102–103	21	
t322	1,3,3-Trimethoxy- propane	CH ₃ OCH ₂ CH ₂ - CH(OCH ₃) ₂	134.18	1,820	0.942	1.4004 ²⁰		45– 46 ^{17mm}		
t323	(Trimethoxysilyl)- propyldiethylene- triamine	(CH ₃ O) ₃ Si(CH ₂) ₃ NH- CH ₂ CH ₂ NHCH ₂ CH ₂ NH ₂	265.4		1.03 ²⁰	1.463 ²⁰				
t324	N-[3-Trimethoxy-silyl)propyl]-ethylenediamine	(CH ₃ O) ₃ Si(CH ₂) ₃ NH- CH ₂ CH ₂ NH ₂	222.4		1.010	1.4450 ²⁰		146 ^{15mm}	>112	
t325	N-(Trimethoxysilyl- propyl)imidazole		230.3		1.00_4^{20}	1.45 ²⁵				
t326	3-(Trimethoxysilyl)- propyl methacrylate	$(CH_3O)_3SiCH_2CH_2$ - $CH_2OOCC(CH_3)$ = CH_2	249.3		1.045420	1.429 ²⁵		190	92	

t327	Trimethylaluminum	(CH ₃) ₃ A1	72.09	4, 643	0.752^{20}	1.43212	15.4	20 ^{8mm}	pyro- phoric	s alk; v sl s alc
t328	Trimethylamine	(CH ₃) ₃ N	59.11	4, 43	0.636		-117.1	2.9	-6	41 aq; misc alc; s bz, chl, eth
t329	Trimethylamine- <i>N</i> -oxide	(CH ₃) ₃ N(O)	75.11				257			s aq, MeOH
t330	2,4,6-Trimethyl- aniline	$(CH_3)_3C_6H_2NH_2$	135.21	12, 1160	0.963	1.5510^{20}		233	96	
t331	1,3,3-Trimethyl-6- azabicyclo[3.2.1]- octane		153.27		0.902	1.4716 ²⁰		194	75	
t332	3,3,5-Trimethyl-1- azacycloheptane		141.26		0.852	1.4563 ²⁰		180	67	
t333	1,2,3-Trimethyl- benzene	$C_6H_3(CH_3)_3$	120.20	5, 399	0.894_4^{20}	1.5139 ²⁰	-25.4	176.1	48	i aq; s alc, eth
t334	1,2,4-Trimethyl- benzene	$C_6H_3(CH_3)_3$	120.20	5, 400	0.8756_4^{20}	1.5048 ²⁰	-43.9	169.4	48	s alc, bz, eth
t335	1,3,5-Trimethyl- benzene	$C_6H_3(CH_3)_3$	120.20	5, 406	0.8637_4^{20}	1.4994 ²⁰	-44.7	164.7	44	misc alc, bz, eth

Trimellitic acid, b29 Trimesic acid, b30 Trimesoyl chloride, b32 Trimethylacetaldehyde, d596 Trimethylacetamide, d597 Trimethylacetic acid, d598 Trimethylacetic anhydride, d599 Trimethylacetyl chloride, d600 endo-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-o1, b216

1.30

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t336	Trimethyl 1,2,4- benzenetricar- boxylate	C ₆ H ₃ (COOCH ₃) ₃	252.22	91, 429	1.261	1.5214 ²⁰	38–40	194 ^{12mm}	>112	
t337	2,2,3-Trimethyl- butane	(CH ₃) ₂ CHC(CH ₃) ₃	100.20	1 ² , 121	0.6901_4^{20}	1.3894 ²⁰	-24.9	80.9		s alc, eth
t338	2,3,3-Trimethyl- 2-butanol	(CH ₃) ₃ CC(CH ₃) ₂ OH	116.20	1 ² , 447	0.8380_4^{25}	1.4233 ²²	15–17	130.5		misc alc, eth
t339	1,1,3-Trimethyl- cyclohexane	$C_6H_9(CH_3)_3$	126.24			1.4296 ²⁰		136.6		
t340	3,5,5-Trimethyl- cyclohex-2-ene- 1-one		138.2	7,65	0.925_{20}^{20}	1.478 ²⁰	-8.1	215.2	96	1.2 aq
t341	2,2,6-Trimethyl- 1,3-dioxen-4-one		142.15	19 ³ , 1604	1.088	1.462220	12–13	65- 67 ^{2mm}		
t342	4,4'-Trimethylene- bis-(1-methyl- piperidine)		238.42		0.896	1.4820 ²⁰	13	215 ^{50mm}	110	
t343	4,4'-Trimethylenedi- piperidine		210.37				65–68			
t344	4,4'-Trimethylenedi- pyridine		198.27				57–60			
t345	Trimethylene oxide		58.08	17,6	0.8930_4^{25}	1.3895 ²⁵		50	<1	misc aq
t345a t346	Trimethylene sulfide 2,2,5-Trimethyl-	(CH ₃) ₂ CHCH ₂ CH ₂ -	74.15 128.26	17 ¹ , 3 1 ³ , 516	$ \begin{array}{c c} 1.025^{20} \\ 0.7072^{20} \end{array} $	$ \begin{array}{c} 1.5102^{20} \\ 1.3997^{20} \end{array} $	-73.3 -105.8	95.0 124.1	<1	v s org solv
t347	hexane 3,5,5-Trimethyl-	C(CH ₃) ₃ (CH ₃) ₃ CCH ₂ CH(CH ₃)-	144.25		0.8236420	1.4300 ²⁵	<-70	194		s alc, eth
t348	1-hexanol Trimethylhydro- quinone	CH ₂ CH ₂ OH (CH ₃) ₃ C ₆ H(OH) ₂	152.19	6, 931			172–174			s aq; v s alc, bz, eth

t348a	2,6,8-Trimethyl- 4-nonanol	(CH ₃) ₂ CHCH ₂ CH(CH ₃)- CH ₂ CH(OH)CH ₂ -	186.33		0.8193		225	93	
		CH(CH ₃) ₂							
t349	2,6,8-Trimethyl-4-	(CH ₃) ₂ CHCH ₂ CH(CH ₃)-	184.31		0.818_{20}^{20}	-75	218.4		
	nonanone	$CH_2C(O)CH_2CH(CH_3)_2$							
t350	α -(-)-1,3,3-Tri-		154.25	6, 70	0.9641_4^{20}	48	201	73	s alc, eth
	methyl-2-								
	norbornanol								

Trimethyl borate, t319
Trimethylchlorosilane, c255 $\alpha, \alpha, 4$ -Trimethyl-3-cyclohexene-1-methanol, t7
3,5,5-Trimethylcyclohex-2-en-1-one, i82
1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid, c5

Trimethylene chlorobromide, b257 Trimethylene chlorohydrin, c214 Trimethylenediamine, p193 Trimethylene dibromide, d93 Trimethylene glycol, p195 Trimethylethylene, m159 Trimethylgermanium bromide, b363 3,3,5-Trimethylhexahydroazepine, t332

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t351	(+)-1,3,3-Tri- methyl-2-norbor- nanone		152.24	7,96	0.94818	1.463518	5–6	192–193	52	v s alc, eth
t352	Trimethyl orthoacetate	CH ₃ C(OCH ₃) ₃	120.15	1 ² , 128	0.9428_4^{25}	1.3859 ²⁵		105		v s alc, eth
t353	Trimethyl orthoformate	HC(OCH ₃) ₃	106.12	2, 19	0.9676_4^{20}	1.3790^{20}		100.6	15	
t354	2,4,4-Trimethyl- 1-oxazoline		113.16		0.887	1.4213 ²⁰		112–113	12	
t355	2,2,3-Trimethyl- pentane	(CH ₃) ₃ CCH(CH ₃)- CH ₂ CH ₃	114.23	11,62	0.7160_4^{20}	1.4030^{20}	-112.3	109.8		s eth; sl s alc
t356	2,2,4-Trimethyl- pentane	(CH ₃) ₂ CHCH ₂ C(CH ₃) ₃	114.23	1 ² , 127	0.6919_4^{20}	1.3915 ²⁰	-107.4	99.2	-7	s bz, chl, eth
t357	2,3,4-Trimethyl- pentane	(CH ₃) ₂ CH[CH(CH ₃)] ₂ CH ₃	114.24	$1^3,500$	0.7190_4^{20}	1.4042^{20}	-109.2	113.5		s alc, org solv
t358	2,2,4-Trimethyl- 1,3-pentanediol	(CH ₃) ₂ CHCH(OH)- C(CH ₃) ₂ CH ₂ OH	146.22	1 ³ , 2225	0.928_{15}^{55}	1.451315	46	229	113	1.8 aq; 75 alc; 22 bz; 25 acet
t359	2,4,4-Trimethyl- 1-pentene	$(CH_3)_3CCH_2$ - $C(CH_3)=CH_2$	112.22	1 ³ , 849	0.7150_4^{20}	1.4112^{20}	-93	101.4	<1	
t360	2,3,5-Trimethyl- phenol	$(CH_3)_3C_6H_2OH$	136.19	6, 518			92–95	230–231		
t361	2,3,6-Trimethyl- phenol	$(CH_3)_3C_6H_2OH$	136.19				62–64			
t362	2,4,6-Trimethyl- phenol	$(CH_3)_3C_6H_2OH$	136.19	6, 158			68–71	220		
t363 t364	Trimethyl phosphate Trimethyl phosphite	(CH ₃ O) ₃ P(O) (CH ₃ O) ₃ P	140.08 124.08	1, 286 1, 285	1.197 1.046 ₄ ²⁰	$1.3958^{20} 1.4080^{20}$	-46 <-78	197 111–112	none 40	100 aq; s alc d aq; misc alc, acet, bz, PE

t365	Trimethyl phos-	(CH ₃ O) ₂ P(O)CH ₂ -	182.11		1.125	1.4370^{20}		118 ^{0.85mm}	>112	
	phonoacetate	COCH ₃				25				
t366	1,2,4-Trimethyl-		128.22		0.851_{25}^{25}	1.4480^{25}	< -50	151 ^{746mm}		s aq, alc, acet, bz
	piperazine									
t367	2,4,6-Trimethyl- pyridine	$(C_5H_2N)(CH_3)_3$	121.18	20, 250	0.9166_4^{22}	1.4979 ²⁰	-43	170.5	57	3.5 aq; misc eth; s alc, bz, chl
t368	N-(Trimethylsilyl)- acetamide	CH ₃ CONHSi(CH ₃) ₃	131.25				52–54	185–186	57	
t369	N-(Trimethylsilyl)- aniline	(CH ₃) ₃ SiNHC ₆ H ₅	165.3		0.940_4^{20}	1.522 ²⁰		207–208		
t370	Trimethylsilyl bromoacetate	BrCH ₂ COOSi(CH ₃) ₃	211.14		1.284	1.4421 ²⁰		57– 58 ^{9mm}	28	
t371	N-(Trimethylsilyl)- diethylamine	$(CH_3)_3SiN(C_2H_5)_2$	145.33					127 ^{738mm}		
t372	2-(Trimethylsilyl)- ethanol	(CH ₃) ₃ SiCH ₂ CH ₂ OH	118.25		0.825	1.4246 ²⁰		71– 73 ^{35mm}	50	
t373	N-(Trimethylsilyl)- imidazole		140.26		0.956	1.4751 ²⁰		99 ^{14mm}	80	
t374	3-(Trimethyl-silyloxy)allene	(CH ₃) ₃ SiOCH ₂ CH=CH ₂	130.3		0.7830_4^{30}	1.4075 ²⁵		100–102		

Trimethylolpropane, e156 Trimethylsilyl cyanide, c298 Trimethylsilyldiethylamine, d343 Trimethylsilyl iodide, i55 Trimethylsilylnitrile, c298

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t375	Trimethylsilyl-	(CH ₃) ₃ SiOC ₆ H ₅	166.3		0.9256420	1.478220	-55	81 ^{23mm}		
t376	phenoxide Trimethylsilyl trifluoroacetate	(CH ₃) ₃ SiOOCCF ₃	186.2		1.077_4^{20}	1.3880 ²⁰		89–90		
t377	Trimethylsulfonium iodide	[(CH ₃) ₃ S]I	204.07				215–220	subl		
t378	Trimethylsulf- oxonium iodide	[(CH ₃) ₃ S(O)]I	220.07				175 d			
t379	Trimethylvinyl- oxysilane	(CH ₃) ₃ SiOCH=CH ₂	116.2		0.772_4^{20}	1.389 ²⁰		74–75		
t380	Trimethylvinyl-	(CH ₃) ₃ SiCH=CH ₂	100.2		0.690_4^{20}	1.3920 ²⁰		55	<1	
t381	2,4,6-Trinitro- aniline	$(O_2N)_3C_6H_2NH_2$	228.12	12, 763	1.76214		188–190	explodes		s hot acet; sl s alc
t382	1,2,4-Trinitro- benzene	$C_6H_3(NO_2)_3$	213.11	5, 271	1.7316		61–62	explodes		5.5 alc; 7.1 eth; i
t383	1,3,5-Trinitro- benzene	$C_6H_3(NO_2)_3$	213.11	5, 271	1.688420		122.5	explodes		0.035 aq; 1.9 alc; 1.5 eth; 6.2 bz
t384	2,4,7-Trinitro-9- fluorenone		315.20	$7^2,410$			175–176			v s bz, acet; sl s aq
t385	Trinitromethane	HC(NO ₂) ₃	151.04	1, 79	1.597_4^{24}		15	47 ^{22mm}		s aq, alk
t386	2,4,6-Trinitro- toluene	$(O_2N)_3C_6H_2CH_3$	227.13	5, 347	1.654_4^{20}		80.1	explodes		1.5 alc; 4 eth; s bz, acet; 0.01 aq
t387	Trioctylamine	[CH ₃ (CH ₂) ₇] ₃ N	353.68	4, 196	0.809	1.4485 ²⁰		365-367	>112	•
t388	s-Trioxane		90.08	19, 381	1.17065		64	115	45	17.2 aq; v s alc, bz, eth, EtAc
t389	Tripentaerythritol		372.41				245 d			
t390	2,4,6-Triphenoxy- s-triazine		357.37				232–234			

t391	Triphenoxyvinyl-silane	$(C_6H_5O)_3SiCH=CH_2$	334.5		1.130_4^{25}	1.562 ²⁵		210 ^{7mm}		
t392	Triphenylamine	(C ₆ H ₅) ₃ N	245.33	12, 181	0.774_0^0		125–127	347–348		s acet, eth; sl s alc
t393	Triphenylantimony	$(C_6H_5)_3Sb$	353.07	16, 891	1.4343 ²⁵		52-54	377		v s bz, eth; sl s alc
t394	Triphenylarsine	$(C_6H_5)_3As$	306.24	16, 828	1.222548	1.6139^{48}	60-62	233 ^{14mm}		v s bz, eth; s alc
t395	1,3,5-Triphenyl-	$(C_6H_5)_3C_6H_3$	306.41	5, 737	1.205		172-174	460		v s bz; s abs alc,
	benzene									eth
t396	Triphenylene		228.29	5,720	1.302		199	425		s alc; v s bz, eth
t397	Triphenylmethane	(C ₆ H ₅) ₃ CH	244.34	5, 698	1.0134_4^{99}		93.4	360		v s hot alc, eth; 49
										chl; 7 bz; s PE;
										i aq
t398	Triphenylmethanol	(C ₆ H ₅) ₃ COH	260.34	6,713	1.199_4^0		164.2	360		v s alc, bz, eth; i aq
t399	Triphenyl phosphate	$(C_6H_5O)_3P(O)$	326.29	6, 179			49-51	244 ^{10mm}	223	misc alc; s bz,
										acet, chl, eth; i
										aq

2,4,6-Trinitrophenol, p173 Triolein, g22 Trioxymethylene, t388 Tripalmitin, g23 Triphenylmethyl bromide, b366

t390

t.396

$$O_2N$$
 O_2
 O_2N
 O_3
 O_4
 O_5
 O_5
 O_5
 O_6
 O_7
 O_8
 $O_$

1.38

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t400	Triphenylphosphine	(C ₆ H ₅) ₃ P	262.29	16,759	1.075481		80.5	377	181	v s eth; s bz, chl, HOAc; sl s alc; i aq
t401	Triphenylphosphine selenide	$(C_6H_5)_3P(Se)$	341.25				187–189			1
t402	Triphenylphosphine sulfide	$(C_6H_5)_3P(S)$	294.36	16, 784			162–164			
t403	Triphenyl phosphite	$(C_6H_5O)_3P$	310.29	6, 177	1.184_{15}^{25}	1.5903 ²⁰	22–24	360	218	s alc, bz, chl, eth
t404	Triphenylsilane	$(C_6H_5)_3SiH$	260.41	$16^2,605$			42–44	152 ^{2mm}		
t405	Tripiperidino- phosphine oxide		299.40	20, 88			40–42	273 ^{50mm}		
t406	Tripropoxyborane	(CH ₃ CH ₂ CH ₂ O) ₃ B	188.08	1 ² , 369	0.8576_4^{20}	1.3948^{20}		175		v s alc; misc eth
t407	Tripropylamine	(CH ₃ CH ₂ CH ₂) ₃ N	143.27	4, 139	0.753	1.4160^{20}	-93	155–158	36	s aq, alc, eth
t408	Tripropylene glycol	H(OCH ₂ CH ₂ CH ₂) ₃ OH	192.3		1.018	1.442^{25}		267.2	141	s aq
t409	Tripropylene glycol butyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ - (CH ₂) ₃ CH ₃	248.4		0.934_{25}^{25}	1.430 ²⁵		276	135	
t410	Tripropylene glycol ethyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ - CH ₂ CH ₃	220.3		0.0948_{25}^{25}	1.427 ²⁵		486	132	
t411	Tripropylene glycol isopropyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ - CH(CH ₃) ₂	234.8		0.0942_{25}^{25}	1.428 ²⁵		112.7	124	
t412	Tripropylene glycol- methyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ CH ₃	206.3		0.967_{25}^{25}	1.42825	-42	242.4	127	misc aq, alc, eth
t413	Tripropyl orthoformate	HC(OCH ₂ CH ₂ CH ₃) ₃	190.28		0.8805_4^{20}	1.407220		108 ^{5mm}		
t414	Tris(butoxyethyl) phosphate	$(C_4H_9OCH_2CH_2O)_3P(O)$	398.48		1.006	1.4359 ²⁰		228 ^{4mm}	>112	
t415	Tris(2-chloro- ethoxy)silane	(CICH ₂ CH ₂ O) ₃ SiH	267.6		1.2886420	1.4577 ²⁰		118 ^{2mm}		

t416	Tris(2-chloro-	(ClCH ₂ CH ₂ O) ₃ P(O)	285.49	$1^2, 337$	1.390	1.4721^{20}		330	232	
t417	ethyl) phosphate Tris(2-chloro- ethyl) phosphite	(CICH ₂ CH ₂ O) ₃ P	269.49		1.353420	1.4863 ²⁰		115 ^{2mm}	190	misc alc, bz, eth
t418	Tris(2,6-dichloro- phenyl) phosphate	$(Cl_2C_6H_3O)_3P(O)$	533.09				208–210			
t419	Tris(dimethylamino)- methane	CH[N(CH ₃) ₂] ₃	145.25		1.4360 ²⁰		42- 43 ^{12mm}			
t420	Tris(dimethylamino)- methylsilane	[(CH ₃) ₂ N] ₃ SiCH ₃	175.4		0.850_4^{22}	1.432 ²²	-11	56 ^{17mm}		
t421	Tris(2-ethylhexyl) phosphite	[CH ₃ (CH ₂) ₃ CH(CH ₂ CH ₃)- CH ₂ O] ₃ P	418.6		0.902_4^{20}	1.4494 ²⁰		164 ^{0.3mm}	185	i aq
t422	Tris(heptafluoro- propyl)-s-triazine	2 -3	585.1		1.7158 ²⁵	1.7158 ²⁵		165		
t423	Tris(hydroxy- methyl)amino- methane	(HOCH ₂) ₃ CNH ₂	121.14	4, 303			172	220 ^{10mm}		

Triphenylsilyl azide, a320 Tripropyl borate, t406 Tripropylsilyl chloride, c258 TRIS, t423 Tris(dimethylamino)silyl chloride, c257a 1,1,1-Tris(hydroxymethyl)ethane, h141

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t424	2-[Tris(hydroxy- methyl)methyl- amino]-1-ethane- sulfonic acid	(HOCH ₂) ₃ CNHCH ₂ - CH ₂ SO ₃ H	229.25				223–225			
t425	1,1,1-Tris(hydroxy- methyl)ethane	CH ₃ C(CH ₂ OH) ₃	120.15	1,520						
t426	3-[N-Tris(hydroxy- methyl)methyl- amino]- 2-hydroxypropane- sulfonic acid	(HOCH ₂) ₃ CNHCH ₂ - CH(OH)CH ₂ SO ₃ H	259.3				226			
t427	3-[Tris(hydroxy- methyl)-methyl- amino]- 1-propanesulfonic acid	(HOCH ₂) ₃ CNHCH ₂ CH ₂ - CH ₂ SO ₃ H	243.28				240 d			
t428	N-[Tris(hydroxy- methyl)methyl]- glycine	(HOCH ₂) ₃ CNHCH ₂ COOH	179.17				184 d			
t429	Tris(2-methoxy- ethoxy)methyl- silane	CH ₃ Si(OCH ₂ CH ₂ OCH ₃) ₃	268.4		1.045 ²⁰	1.420 ²⁰		145 ^{16mm}		
t430	Tris(2-methoxy- ethoxy)vinylsilane	H ₂ C=CHSi(OCH ₂ - CH ₂ OCH ₃) ₃	280.38		1.034_4^{25}	1.427 ²⁵		284–286	65	
t431	Tris(2-methylallyl)- amine	$[H_2C = C(CH_3)CH_2]_3N$	173.91	$4^3,462$	0.794	1.4575 ²⁰		83– 85 ^{15mm}	53	
t432	Tris(pentafluoro- ethyl)-s-triazine		435.1		1.6506 ²⁵	1.3131 ²⁵		121–122		

t433 t434 t435	1,3,5-Trithiane Trithiocarbonic acid 1,2,4-Trivinylcyclo-	(HS) ₂ C(S) (H ₂ C=CH) ₃ C ₆ H ₉	138.27 110.21 162.28	19, 382 3, 221	1.483 ²⁰ 0.836	$1.8225^{20} \\ 1.4780^{20}$	216–218 –26.9	57.8 88 ^{20mm}	68	s bz; sl s alc, eth d aq, alc; sl s eth
t436	hexane L-(-)-Tryptophan		204.23	22, 546			280–285 d			1 aq; s hot alc, alk; i eth, chl
t437	L-Tyrosine	(HO)C ₆ H ₄ CH ₂ - CH(NH ₂)COOH	181.19	14, 605			>300 d			0.03 aq; 0.01 alc; s alk; i eth
t438	L-Tyrosine hydrazide	HOC ₆ H ₄ CH ₂ CH(NH ₂)- CONHNH ₂	195.22	14 ¹ , 665			196–198			
u1	Undecanal	CH ₃ (CH ₂) ₉ CHO	170.30	1,712	0.825	1.4322^{20}	-4	115 ^{5mm}	96	i aq; s alc, eth
u2	Undecane	CH ₃ (CH ₂) ₉ CH ₃	156.31	1, 170	0.7402_4^{20}	1.4173^{20}	-25.6	195.9	60	i aq; misc alc, eth
u3	Undecanoic acid	CH ₃ (CH ₂) ₉ COOH	186.30	2,358	0.8907	1.4294^{45}	28.5	228 ^{160mm}		s alc, chl, eth; i aq
u4	1-Undecanol	CH ₃ (CH ₂) ₁₀ OH	172.31	1,427	0.8324^{20}	1.4402^{20}	15.9	242.8	>112	0.02 aq; s alc
u5	2-Undecanone	CH ₃ (CH ₂) ₈ COCH ₃	170.30	1, 173	0.829	1.4280 ²⁰	11–12	231–232	88	s alc, bz, chl, eth, acet; i aq
u6	6-Undecanone	CH ₃ (CH ₂) ₄ - CO(CH ₂) ₄ CH ₃	170.30	1, 174	0.831	1.4280 ²⁰	14.6	228	88	i aq; v s alc, eth
u7	10-Undecenal	H ₂ C=CH(CH ₂) ₈ CHO	168.28		0.810	1.4427^{20}			92	
u8	1-Undecene	$CH_3(CH_2)_8CH = CH_2$	154.29	1, 225	0.763_4^{20}	1.426120	-49.2	192.7		i aq; misc alc, eth

Tris(7-methylnonyl) phosphite, t308 Trityl alcohol, t398 Tryptamine, a170 Tyramine, a173 Umbelliferone, h109 Undecyl alcohol, u4

Undecyl-10-en-1-oic acid, u9 Undecylenic aldehyde, u7 Undecylic aldehyde, u1

TABLE 1.15 Physical Constants of Organic Compounds (continued)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
u9	10-Undecenoic acid	H ₂ C=CH(CH ₂) ₈ COOH	184.28	2, 458	0.907_4^{24}	1.449320	24.5	137 ^{2mm}	148	s alc, chl, eth; i aq
u10	10-Undecen-1-ol	H ₂ C=CH(CH ₂) ₉ OH	170.30	1,452	0.850^{15}	1.4500^{20}	-2	245	93	
u11	10-Undecenoyl chloride	H ₂ C=CH(CH ₂) ₈ COCl	202.73	2, 459	0.944	1.453220		122 ^{10mm}	93	
u12	Urea	(H ₂ N) ₂ CO	60.06	3, 42	1.32_4^{18}		132.7	d>mp		100 aq; 20 alc
u13	Uric acid		168.11	26, 513	1.893^{20}		>300	d		s alk; i aq, alc, eth
u14	Uridine		244.20	31, 23			165			s aq; hot alc, pyr
v1	L-Valine	(CH ₃) ₂ CH- CH(NH ₂)COOH	117.15	4, 427	1.230		315	subl		8.8 aq; v sl s alc, eth
v2	Vinyl acetate	H ₂ C=CHOOCCH ₃	86.09	21,63	0.9318_4^{20}	1.3959^{20}	-92.8	72.5	-6	2 aq; misc alc, eth
v3	5-Vinylbicyclo- [2.2.1]-2-heptene		120.19		0.84	1.4802	-80	141		
v4	Vinyl crotonate	CH ₃ CH=CHCOOCH=CH ₂	112.13	2^3 , 1263	0.940	1.4488^{20}		50 ^{10mm}	27	
v5	Vinylcyclohexane	$C_6H_{11}CH=CH_2$	110.20	5 ¹ , 35		1.446320		128	21	
v6	4-Vinyl-1-cyclohexene		108.18	51,63	0.830_4^{20}	1.4640^{20}	-101	126-127	20	
v7	1-Vinylimidazole		94.12	23 ⁴ , 569	1.039	1.5308 ²⁰		78– 79 ^{13mm}	81	
v8	5-Vinyl-2- norbornene		120.20		0.8411	1.4802 ²⁰	-80	141	27	
v9	2-Vinylpyridine	$(C_5H_4N)CH=CH_2$	105.14	20, 256	0.975	1.5490^{20}		158-159	43	v s alc, chl, eth
v10	4-Vinylpyridine	$(C_5H_4N)CH=CH_2$	105.14	$20^2, 170$	0.975	1.5500^{20}		65 ^{15mm}	51	sl s hot aq, hot alc
v11	N-Vinyl-2- pyrrolidinone		111.14		0.980	1.5120 ²⁰		93 ^{13mm}	93	_
x1	Xanthene		182.22	17,73			101	310–312		s bz, eth; sl s alc,
x2	Xanthen-9- carboxylic acid		226.23	$12^2, 279$			217 d			s hot alc, eth
x3	9-Xanthenone		196.21	17, 354			174	350 ^{730mm}		0.5 alc; v s chl

Uracil, p268
5-Ureidohydantoin, a77
Urethane, e91
Valeraldehyde, p27
Valeric acid, p36
γ-Valerolactone, p40
Valerone, d531
Valeronitrile, p33
Valeryl chloride, p44
Valinols, a213, a214

Vanillic acid, h132 Vanillin, h131 o-Vanillin, h130 Vanillyl alcohol, h135 Veratraldehyde, d430 Veratric acid, d434 Veratrole, d431 Veronal, d280 Vinylacetic acid, b403 Vinyl bromide, b284 Vinyl 2-butenoate, v4
Vinyl chloride, c109
Vinylidene chloride, d178
Vinyltrimethylsilane, t380
Vinyltris (2-methoxyethoxy)silane, t430
Vitamin B₁, t139
Vitamin B₂, r4
Vitamin C, a312
Xanthone, x3

CH₂=CH

v8

CH=CH₂

v11

x1

COOH

x2

1.393

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
x4	o-Xylene	C ₆ H ₄ (CH ₃) ₂	106.17	5, 362	0.8802_4^{20}	1.5054 ²⁰	-25.2	144.4	32	misc alc, eth;
x5	m-Xylene	C ₆ H ₄ (CH ₃) ₂	106.17	5, 370	0.8684415	1.4972 ²⁰	-47.9	139.1	25	0.017 aq misc alc, eth; 0.02
x6	p-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 382	0.8611_4^{20}	1.495820	13.3	138.4	30	v s eth; s alc; 0.02
x7 x8	Xylitol D-(+)-Xylose	HOCH ₂ (CHOH) ₃ CH ₂ OH	152.15 150.13	1,531 31,47	1.535°		95–97 144–145			aq s aq 117 aq; s hot alc,
x9	<i>m</i> -Xylylenediamine	$C_6H_4(CH_2NH_2)_2$	136.20	13, 186	1.032	1.5709 ²⁰		265 ^{745mm}	>112	pyr

Xylene- α , α' -diol, b18 Xylenols, d579, d580, d581, d582, d583, d584 *o*-Xylyl bromide, b368 Xylyl chlorides, c258, c259, c260 *p*-Xylylene glycol, b18

SECTION 2

INORGANIC AND ORGANOMETALLIC COMPOUNDS

Table 2.1 Physical Constants of Inorganic Compounds								2	2.2	2
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2.2 SECTION 2

This section summarizes the properties of various chemical compounds commonly encountered in organic chemistry that are often referred to either as inorganic or organometallic. In some cases, the distinction is artificial and the reader should refer to Section 1 if the expected compound is not presented here. Most compounds containing metals are collected here, rather than in Section 1.

TABLE 2.1 Physical Constants of Inorganic Compounds

Explanation of column headings

Names, while following the IUPAC nomenclature, are generally alphabetized by the central atom to facilitate their location. An example of the table organization is given below for Al_3C_4 , aluminum tetracarbide. It is entered in Table 2.1 as follows:

Main headingAluminumSubgroupingcarbideActual table listingAluminum

(tetra-) carbide (tri-)

Solvates are listed under the entry for the anhydrous salt. Hydrazine hydrate, $H_2N - NH_2 \cdot H_2O$ is listed under hydrazine. Magnesium sulfate heptahydrate (epsom salt) is listed under **Magnesium**, using the subgroup sulfate 7-water. Inorganic acids are entered under hydrogen, For example, HF is listed under **Hydrogen**, using the subgroup fluoride. Where an elemental designation would be confusing or inappropriate, the compound is listed alphabetically as in the case of **hydroxylamine**, HONH₂.

Abbreviations used in the Table

ca, approximately	g, gas	pyr, pyriaine
chl, chloroform	glyc, glycerol	s, soluble
conc, concentrated	h, hot	satd, saturated
cub, cubic	hex, hexagonal	sl, slightly
d, decompose(s)	hyd, hydrolysis	soln, solution
dil, dilute	i, insoluble	solv, solvent(s)
DMF,	ign, ignites	subl, sublimes
dimethylformamide	lq, liquid	tetr, tetragonal
eth, diethyl ether	MeOH, methanol	THF, tetrahydrofuran
EtOH, ethanol	min, mineral	tr, transition
expl, explodes,	misc, miscible	v, very
explosive	org, organic	vac, vacuo or vacuum
fcc, face-centered cubic	PE, petroleum ether	viol, violently
	chl, chloroform conc, concentrated cub, cubic d, decompose(s) dil, dilute DMF, dimethylformamide eth, diethyl ether EtOH, ethanol expl, explodes, explosive	chl, chloroform conc, concentrated cub, cubic d, decompose(s) dil, dilute DMF, dimethylformamide eth, diethyl ether EtOH, ethanol expl, explodes, explosive glyc, glycerol h, hot hex, hexagonal hyd, hydrolysis i, insoluble ign, ignites lq, liquid MeOH, methanol min, mineral expl, explodes, explosive glyc, glycerol hex, hexagonal hyd, hydrolysis i, insoluble ign, ignites lq, liquid min, mineral min, mineral expl, explodes, explosive org, organic

Formula Weights are based on the International Atomic Weights of 1973 and are computed to the nearest hundredth of an a.m.u.

Density values are given at room temperature unless otherwise indicated by a superscript figure indicating a temperature in °C. Thus, 2.487^{15} indicates a density of 2.487 for the named substance at 15 °C. For gases density values are given in grams per liter ($g \cdot L^{-1}$).

Melting Point values are recorded in $^{\circ}$ C. In certain cases decomposition is indicated with the letter "d" that either precedes or follows the number. The value 250 d indicates that the substance melts at 250 $^{\circ}$ C with decomposition. The value d 250 indicates that decomposition only occurs at 250 $^{\circ}$ C and higher temperatures. Where a value such as " $^{-}$ 6H₂O, 150" is given, it indicates a loss of 6 moles of water per formula weight of the compound at a temperature of 150 $^{\circ}$ C.

Boiling Point values are given at atmospheric pressure (760 mm of mercury) unless otherwise indicated; a value of 82 means that the boiling point is 82 °C at 760 mm Hg. A value of 82 15 means that the boiling point is 82 °C when the pressure is 15 mmHg. The specification "subl 550" indicates that the compound sublimes at 550 °C.

Solubility is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent. If the solvent is unspecified, it is water. If no temperature is specified, the solubility is for the substance at room temperature. Other temperatures (in °C) are indicated by superscript. The symbols of the common mineral acids represent aqueous solutions of those acids.

TABLE 2.1 Physical Constants of Inorganic Compounds

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Aluminum	Al	26.98	2.70	660.1	2450	s HCl, H ₂ SO ₄ , alk
acetylacetonate	$Al(C_5H_7O_2)_3$	324.31	1.27	subl 193 (vac)	314	i aq; v s alc; s bz, eth
ammonium bis(sulfate) 12-water	AlNH ₄ (SO ₄) ₂ •12H ₂ O	453.33	1.64	$-12 H_2O, 250$	d>280	15 aq; i alc
bis(acetylsalicylate)	Al(OOCC ₆ H ₄ O- COCH ₃) ₂ OH	402.30				v sl s aq, alc, eth
bromide	AlBr ₃	266.71	2.6410	97.5	253.3	d viol aq; s alc, acet, bz CS ₂
butoxide, sec-	$Al(C_4H_9O)_3$	246.33	0.967		200-206 ^{30 mm}	v s org solv (flash point 27°C)
butoxide, tert-	$Al(C_4H_9O)_3$	246.33	1.025_0^{20}	subl 180		v s org solv
(tetra-) carbide, tri-	Al_4C_3	143.96	2.36	2100	d>2200	d to CH ₄ in aq (fire hazard)
chlorate	Al(ClO ₃) ₃	277.35				v s aq; s alc
chloride	AlCl ₃	133.34	2.44	194 ^{2.5} atm	subl 181	70 aq (viol); 100 ¹² abs alc; s CCl ₄ , eth; sl s bz
chloride 6-water	AlCl ₃ •6H ₂ O	241.43	2.40	d 100		83 ²⁰ aq; 25 abs alc; s eth
ethoxide	$Al(C_2H_5O)_3$	162.14	1.42_0^{20}	134	205 ^{14 mm}	s hot aq (d); v sl a alc, eth
fluoride	AlF3	83.98	2.882_4^{25}	1040	subl 1276	0.562 ⁵ aq; i a, alk, alc, acet
hydroxide	Al(OH) ₃	78.00	2.42	$-H_2O, 300$		i aq; s a,alk
iodide	AlI ₃	407.71	3.98^{25}	191	360	s aq(d); s alc, CS ² , eth
isopropoxide	$Al(C_3H_7O)_3$	204.25	1.0346_0^{20}	118.5	135 ^{10 mm}	d aq; s alc, bz, chl, PE
nitrate 9-water	Al(NO ₃) ₃ •9H ₂ O	375.13		73	d 135	64 ²⁵ aq; 100 alc; s acet
oxide	Al ₂ O ₃	101.96	3.965	2054	2980	i aq; v sl s a, alk
phenoxide	$Al(C_6H_5O)_3$	306.27	1.23	d 265		d aq; s alc, chl, eth
potassium bis (sulfate 12-water	AlK(SO ₄) ₂ •12H ₂ O	474.39	1.757 ²⁰	$-9H_{2}O, 92$	$-12H_2O, 200$	11.4 ²⁰ aq
propoxide	$Al(C_3H_7O)_3$	204.25	1.0578_0^{20}	106	248 ^{14 mm}	d aq; s alc
sodium bis(sulfate) 12-water	AlNa(SO ₄) ₂ ·12H ₂ O	458.28	1.675 ²⁰	61		110 ¹⁵ aq

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Aluminum						
stearate	Al(C ₁₈ H ₃₅ O ₂) ₃	877.42	1.010	103		i aq; s alc, bz, alk
sulfate	$Al_2(SO_4)_3$	342.15	2.710	d 770		36.4 ²⁰ aq; sl s alc
sulfate 18-water	Al ₂ (SO ₄) ₃ ·18H ₂ O	666.45	1.69^{17}	d 86.5		87º aq; i alc
tetrahydroborate	Al(BH ₄) ₃	71.53		-64.5	44.5	d aq
Amidosulfuric acid	H ₂ NSO ₃ H	97.09	2.126	205	d	14.7 aq
Ammonia	NH ₃	17.03	0.7188^{20}	-77.75	-33.42	89.9 ag; 13.2 ²⁰ alc; s eth, org solv
$-d_3$ or [2 H]	ND ₃ or N ² H ₃	20.05	$\begin{array}{c} \mathbf{g} \cdot \mathbf{L}^{-1} \\ 0.8437^{20} \\ \mathbf{g} \cdot \mathbf{L}^{-1} \end{array}$	-74.33	-31.05	
Ammonium						
acetate	NH ₄ C ₂ H ₃ O ₂	77.08	1.17^{20}	114	d	148 ⁴ aq; 7.9 ¹⁵ MeOH; s alc
benzoate	NH ₄ C ₇ H ₅ O ₂	139.16	1.260	d 198	subl 160	20 ¹⁵ aq; 2.8 alc; s glyc; i eth
boranate, tetrafluoro-	NH ₄ BF ₄	104.84	1.8715	subl		25 ¹⁶ aq
bromide	NH ₄ Br	97.95	2.429	452 (under	d 397 (vac)	76 ²⁰ aq; s acet, alc, eth
				pressure)		_
carbamate	NH ₄ COONH ₂	78.07		subl 60		v s aq; sl s alc; i eth
carbonate 1-water	(NH ₄) ₂ CO ₃ ·H ₂ O	114.10		d 20		100 ¹⁵ aq; i alc
cerate(IV), hexanitrato-	$(NH_4)_2[Ce(NO_3)_6]$	548.23				135 ²⁰ aq; s alc, HNO ₃
chloride	NH₄Cl	53.49	1.527	subl 340		26 ¹⁵ aq; 0.6 ¹⁹ abs alc; i acet, eth
chromate	$(NH_4)_2CrO_4$	152.08	1.9112	d 180		34 ²⁰ aq; sl s MeOH, acet; i alc
chromium(III) bis(sulfate 12-water)NH ₄ Cr(SO ₄) ₂ ·12H ₂ O	478.34	1.72	94		7.2º aq
citrate	$(NH_4)_3C_6H_5O_7$	243.22	1.48	d		100 aq; sl s alc
copper(II) tetrachloride 2-hydrate	Cu(NH ₄) ₂ Cl ₄ ·2H ₂ O	277.46	1.993	$-2H_2O, 110$	d>120	40 ²⁰ aq; s alc
dichromate(VI)	$(NH_4)_2Cr_2O_7$	252.06	2.155_4^{25}	d 170		36 ²⁰ aq; s alc (flammable)

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6-water molybdate(VI)(6-) (NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O 1235.86 2.498 -H ₂ O, 90 d 190 43 aq; s a; i alc
6-water molybdate(VI)(6-) $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ 1235.86 2.498 $-H_2O$, 90 d 190 43 aq; s a; i alc
2 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -
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nitrate NH ₄ NO ₃ 80.04 1.725 ²⁵ 169.6 210 ^{11 mm} 192 ²⁰ aq; 3.8 ²⁰ alc; 17 ²⁰ MeOH
octadecanoate $NH_4OOC(CH_2)_{16}CH_3$ 301.50 21–22 sl s aq; s alc; i acet
octanoate $NH_4OOCC_7H_{15}$ 161.24 $d ext{ on standing}$ $v ext{ s aq, alc, acet; sl s eth}$
oxalate 1-water $(NH_4)_2C_2O_4 \cdot H_2O$ 142.11 1.50 $d.70$ 1.51 1.50 1.51
palladate(II) tetrachloro- $(NH_4)_2PdCl_4$ 284.29 2.170 d v s aq; i abs alc
perchlorate NH_4CIO_4 117.50 1.95 $d 240$ 22^{20} ag; s MeOH; sl s alc, acet
percondisulfate $(NH_4)_2S_2O_8$
phosphate, hexafluoro- NH_4PF_6
phosphiate, inclaim to $\frac{105.00}{100}$ $\frac{2.1004}{100}$ $\frac{100.00}{100}$ $\frac{2.1004}{100}$ $\frac{100.00}{100}$ $\frac{2.1004}{100}$ $\frac{100.00}{100}$
phosphiliate $NH_4C_6H_5N_3O_7$
1
silicate, hexafluoro- $(NH_4)_2SiF_6$ 178.14 2.011 d 18.6 ²⁰ aq; i alc, acet

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Ammonium						
sulfamate	NH ₄ SO ₃ NH ₂	114.13		131	d 160	v s aq; sl s alc
sulfate	$(NH_4)_2SO_4$	132.14	1.769^{20}	d>280		43.5^{25} aq; i alc, acet
sulfide	$(NH_4)_2S$	68.14		d		v s aq; s alc
DL-tartrate	$(NH_4)_2C_4H_4O_6$	184.15	1.601	d		58 ¹⁵ ag; sl s alc
tetraborate 4-water	$(NH_4)_2B_4O_7\cdot 4H_2O$	263.44				s aq; i alc
thiocyanate	NH ₄ SCN	76.12	1.305	149.6	d 170	128° aq; v s alc; s acet
thiosulfate	$(NH_4)_2S_2O_3$	148.20	1.679	d 150		v s aq
vanadate(V)(1-)	NH ₄ VO ₃	116.98	2.326	d 200		$0.48^{\hat{20}}$ aq
Antimony						•
(III) chloride	SbCl ₃	228.11	3.14_4^{20}	73.4	223.5	10 ²⁰ aq; s alc, bz, chl
(V) chloride	SbCl ₅	299.02	2.336_4^{20}	3.5	140	d aq; s HCl, chl, CCl ₄
(III) fluoride	SbF ₃	178.75	4.379_{20}^{20}	292	376	444 ²⁰ aq
(V) fluoride	SbF ₅	216.74	2.99^{23}	8.3	141	d viol aq; s HOAc; forms solids with alc, bz, CS ₂ , eth
hydride	SbH ₃	124.77	4.3615	-91.5	-18.4	20° mL aq; s CS ₂
(III) oxide	Sb ₂ O ₃	291.50	5.2	655	1425	v sl s aq; s HCl, KOH
(V) oxide	Sb_2O_5	323.50	2.78	$-O_2, >300$		v sl s aq; sl s warm KOH, eth
potassium oxide tartrate 0.5-water	K(SbO)C ₄ H ₄ O ₆ •O.5H ₂ O	333.93	2.607	d 100		8.3 ²⁰ aq; 6.7 glyc; i alc
(III) sulfide	Sb ₂ S ₃	339.69	4.64	546		0.002 ²⁰ aq d; s H ₂ SO ₄
(V) sulfide	Sb ₂ S ₅	403.82				i ag; s HCl, d NaOH
Argon	Ar	39.95	1.7824 g·L ⁻¹	-189.38	-185.87	3.36 ²⁰ mL aq
Arsenic	As	74.92	5.72	817 ^{28 atm}	subl 612	i aq; s HNO ₃
(III) chloride	AsCl ₃	181.28	2.1497_4^{25}	-16	130.2	d aq; misc chl, CCl ₄ , eth; s alc
(III) oxide dimer	As_4O_6	395.68	4.15	313	465	1.8 ²⁰ aq; s alc

(V) oxide	As_2O_5	229.84	4.32	d 800		66 ²⁰ aq; s alc
(III) sulfide	As_2S_3	246.04	3.46	300-325	707	i aq; s alk; slowly s hot HCl
Barium						
acetate 1-water	$Ba(C_2H_3O_2)_2 \cdot H_2O$	273.46	2.19	d 150		76 ²⁰ aq; 0.14 alc
benzenesulfonate	$Ba(O_3SC_6H_5)_2$	451.70				s aq; sl s alc
carbonate	BaCO ₃	197.35	4.43	d 1360		0.002 aq; s a
chlorate 1-water	Ba(ClO ₃) ₂ •H ₂ O	322.26	3.18	$-H_2O$, 120	$-O_2, 250$	34 ²⁰ aq
chloride	BaCl ₂	208.25	3.856	962	2029	36 ²⁰ aq
fluoride	BaF ₂	175.34	4.89	1368	2272	0.16^{20} aq
hydrogen phosphate	BaHPO ₄	233.32	4.165^{15}	d 410		0.01 aq; s a
hydroxide 8-water	Ba(OH) ₂ •8H ₂ O	315.48	2.18^{16}	78		3.9 ²⁰ aq
manganate(VI)(2-)	BaMnO ₄	256.28	4.85			v sl s aq
nitrate	Ba(NO ₃) ₂	261.35	3.24	575	d	9 ²⁰ aq
nitrite 1-water	Ba(NO ₂) ₂ ·H ₂ O	247.37	3.173^{20}	d 115		73 ²⁰ aq; i alc
oxide	BaO	153.34	5.72	2013	3088	3.5 ²⁰ aq
perchlorate 3-water	Ba(ClO ₄) ₂ •3H ₂ O	390.29	2.74	d 400		19825 aq; s MeOH; sl s alc, acet
permanganate	Ba(MnO ₄) ₂	375.21	3.77	d 200		62 ¹¹ aq
peroxide	BaO ₂	169.34	4.96	450	$-O_2,800$	1.5° aq
sulfate	BaSO ₄	233.40	4.50^{15}	1580		0.0002 aq
sulfide	BaS	169.40	4.25^{15}	2227		7.9 ²² aq d
sulfite	BaSO ₃	217.40		d		0.02^{20} aq
thiocyanate 2-water	Ba(SCN) ₂ •2H ₂ O	289.53	2.286^{18}	d 160		170 ²⁵ aq
thiosulfate 1-water	BaS ₂ O ₃ ·H ₂ O	267.48	3.5^{18}	d 220		0.21 ²⁰ aq
Beryllium	Be	9.01	1.86	1277	2484	i q; s a, alk
bromide	$BeBr_2$	168.83	3.465^{25}	506-509	521	v s aq; s alc; 19 pyr
chloride	BeCl ₂	79.92	1.899 ²⁵	399	482	42 aq; s alc, eth, CS ₂ , pyr; i bz
fluoride	BeF ₂	47.01	1.986_4^{25}	552	1175	v s aq but slow
hydride	BeH_2	11.03		$-H_2$, 220		d slowly aq; d rapidly a
hydroxide	Be(OH) ₂	43.03	1.92	134 d		s hot conc a, alk
iodide	BeI_2	262.82	4.2	480	482	hyd aq; s alc, eth, CS ₂
oxide	BeO	25.01	3.01	$2408(\alpha)$	3787	s conc H ₂ SO ₄
sulfate 4-water	BeSO ₄ •4H ₂ O	177.14	1.71311	$-4H_2O, 270$	d 580	39 ²⁰ aq; i alc

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Bismuth						
chloride, tri-	BiCl ₃	315.34	4.75	ca 232	447	d aq; s HCl, alc, eth, acet
fluoride, penta-	BiF ₅	303.98	5.4^{25}	151	230	d viol aq giving O ₃
hydroxide	Bi(OH) ₃	260.00	4.36	$-H_2O, 100$		d aq; s a
(III) nitrate 5-water	Bi(NO ₃) ₃ •5H ₂ O	485.07	2.83	d 30		d aq; s, acet
(III) oxide	Bi ₂ O ₃	495.96	8.76	817	1890	i aq; s a
Boron						
bromide, tri-	BBr ₃	250.57	2.695°	-46.0	91.3	d aq
choride, tri-	BCl ₃	117.19	1.35_4^{12}	-107	18	d aq, alc
fluoride, tri-	BF ₃	67.81	$2.99\mathrm{g}\cdot\mathrm{L}^{-1}$	-127.1	-100.4	1050 mL aq; s bz, chl, CCl ₄
fluoride-1-diethyl ether	$BF_3 \cdot O(C_2H_5)_2$	141.94	1.125_4^{25}	-60.4	125.7	d aq
fluoride-1-methanol	BF ₃ •CH ₃ OH	131.89	1.203		$59^{4\mathrm{mm}}$	
oxide	B_2O_3	69.62	2.46	450	2065	sl s aq
Bromine	Br_2	159.81	3.1028	-7.3	58.75	3.6 ²⁰ aq; v s alc, chl, eth, CS ₂
fluoride, tri-	BrF ₃	136.90	2.803^{25}	8.77	125.74	d viol aq; d alk
Cadmium						
acetate	$Cd(C_2H_3O_2)_2$	230.50	2.341	256	d	v s aq
chloride	CdCl ₂	183.32	4.047	568	961	120 ²⁵ aq
iodide	CdI_2	366.21	5.670^{30}	387	796	85 ²⁰ aq; s alc, acet, eth
oxide	CdO	128.40	8.15	subl 1497		i aq; s a
sulfate-water (3/8)	3CdSO ₄ ·8H ₂ O	769.56	3.09	$-H_{2}O, 40$	forms mono-	94.4 ²⁵ ; i alc
					hydrate 80	
sulfide	CdS	144.46	4.82 hex		sub 1380 (in N2)	3.13 ¹⁸ aq; s a
Calcium						
acetate	$Ca(C_2H_3O_2)_2$	158.17	d > 160			37° aq; i alc, acet, bz
arsenate(V)	$Ca_3(AsO_4)_2$	398.08	3.620			0.013^{25} aq

bromide	CaBr ₂	199.90	3.353	765	806-812	143 ₂₀ aq; v s alc, acet
carbide, di-	CaC ₂	64.10	2.22		2300	d aq giving C ₂ H ₂
carbonate	CaCO ₃	100.09	2.930	d 900		0.0013 ²⁰ ; s a
chlorate	Ca(ClO ₃) ₂	206.99		340		178 aq; s alc, acet
chloride	CaCl ₂	110.99	2.15	772	1940	75 ²⁰ ; s alc, acet
chloride 6-water	CaCl ₂ ·6H ₂ O	219.08	1.71	$-6H_2O, 200$		536 ²⁰ aq; s alc
citrate 4-water	$Ca(C_6H_6O_7)\cdot 4H_2O$	570.51		$-4H_2O$, 120		0.85 ¹⁸ aq; 0.0065 ¹⁸ alc
cyanamide	CaCN ₂	80.11	2.29_4^{20}	1340	subl 1150	i aq; no known solv
cyanide	Ca(CN) ₂	92.12	·	d 350		d aq
liphosphate	Ca ₂ P ₂ O ₇	254.10	3.09	1230		i aq; s a
fluoride	CaF ₂	78.08	3.180	1418	2510	0.002^{20} aq; s1 s a
Formate	Ca(OOCH) ₂	130.12	2.015	d		16.6 ²⁰ aq; i alc
glycerophosphate	Ca[C ₃ H ₅ (OH) ₂]PO ₄	210.16		d>170		1.7 ²⁰ aq, i alc
hydrogen phosphate, di-	Ca(H ₂ PO ₄) ₂ ·H ₂ O	252.07	2.220^{18}_{4}	$-H_2O, 109$	d 203	1.8 ³⁰ aq
1-water						
nydroxide	Ca(OH) ₂	74.09	2.24	$-H_2O, 522$		0.17 ¹⁰ aq; s a
nypochlorite	Ca(OCl) ₂	142.99	2.35	100 d		d aq evolving Cl ₂ ; i alc
odate 6-water	Ca(IO ₃) ₂ •6H ₂ O	497.98		d 35		0.24 ²⁰ aq; i alc
actate 5-water	Ca(C ₃ H ₅ O ₃) ₂ •5H ₂ O	308.30		$-3H_2O, 100$	$-5H_2O$, 120	5.4 ¹⁵ aq; v sl s alc
nitrate	Ca(NO ₃) ₂	164.09	2.504^{18}	561		152 ³⁰ aq
nitrite 4-water	Ca(NO ₂) ₂ •4H ₂ O	204.5	1.674_0^0	$-2H_{2}O, 44$		84.5 ¹⁸ ag; sl s alc
oleate	$Ca(C_{18}H_{33}O_{2})_{2}$	603.01	· ·	83–84	d 140	0.04 aq; s bz, chl; v sl s alc
xide	CaO	56.08	3.25	2927	3500	0.13 ²⁵ aq; s a
almitate	Ca(C ₁₆ H ₃₁ O ₂) ₂	550.93		d 155		0.003 aq; sl s bz, chl; i alc, eth
antothenate	Ca[O ₂ CH ₂ CH ₂ HO-	476.55		d 195–196		35 aq; sl s alc, acet
(vitamin B ₃)	CH(OH)C(CH ₃) ₂ -					
3/	CH ₂ OH ₁					
peroxide	CaO ₂	72.08	2.92_4^{25}	d 275		sl s aq; s a
henoxide	$Ca(OC_6H_5)_2$	226.28				sl s aq, alc
hosphate	$Ca_3(PO_4)_2$	310.18	3.14	1730		0.03^{25} ; s a; i alc
alicylate 2-water	Ca(C ₇ H ₅ O ₃) ₂ ·2H ₂ O	350.34		$-2H_{2}O, 120$	d 240	2.8 ¹⁵ aq; 0.015 ¹⁶ EtOH
elenate 2-water	CaSeO ₄ ·2H ₂ O	219.07	2.68^{20}_{4}	$-2H_{2}^{2}O, 200$	d 698	9.2 ²⁵ aq
stearate	$Ca(C_{18}H_{35}O_2)_2$	607.04	-	179–180		0.004 ¹⁵ aq; s hot pyr; i chl, eth

TABLE 2.1 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Calcium						
succinate 3-water	CaC ₄ H ₆ O ₄ ·3H ₂ O	212.22				1.28 ²⁰ aq; s a; i alc
sulfate	CaSO ₄	136.14	2.960	1400		0.20 aq; s a
sulfate hemihydrate	CaSO ₄ •0.5H ₂ O	145.15		-H ₂ O, 163		0.3 ²⁰ aq; s a, glyc
sulfate 2-water	CaSO ₄ •2H ₂ O	172.17	2.32	$-2H_2O$, 163		0.26 ²⁰ aq; s a, glyc
sulfite 2-water	CaSO ₃ •2H ₂ O	156.17		$-2H_2O, 100$		0.004 aq; s a; sl s alc
DL-tartrate 4-water	CaC ₄ H ₄ O ₆ ·4H ₂ O	260.21		$-4H_2O, 200$		0.0045^{25} aq; sl s alc
tetrahydridoaluminate	Ca(AlH ₄) ₂	102.10				ign moist air; d viol aq, alc
thiocyanate 3-water	Ca(SCN) ₂ ·3H ₂ O	210.29		d 160		150 aq; v s alc
Carbon						
(graphite)	C	12.01	2.25^{20}	4000 ^{63.5} atm	3930	i aq, alc
bromide, tetra-	CBr ₄	331.65	3.42	90.1	190	i aq; s alc, chl, eth
chloride, tetra-	CCl ₄	153.82	1.5867_{20}^{20}	-22.9	76.7	i aq; s alc, chl, eth
hydride, tetra-	CH ₄	16.04	0.415^{-164}	-182.48	-161.49	i aq; s bz
iodide, tetra-	CI ₄	519.63	4.34	d 171		sl hyd aq; s alc, bz, eth
oxide, mono-	СО	28.01	0793 (lq) 1.250 g·L ⁻¹ (gas)	-205.05	-191.49	2.1 mL aq; s alc, bz
oxide di-	CO ₂	44.01	1.56 ⁻⁷⁹ (c) 1.975 g•L ⁻¹	-56.2 solid subl	-78.44	31 ¹⁵ mL aq
(tri-) oxide, di-	C_3O_2	68.03	1.114_4^0	-112.19	6.4	d aq to malonic acid
selenide, di-	CSe ₂	169.93	2.663_4^{25}	-43	125.1	i aq; d alc, pyr; misc CCl ₄ ; s acet, eth
sulfide, di-	CS_2	76.14	1.261^{22}	-111.6	46.26	0.29 ²⁰ aq; s alc, eth

Carbonic acid	$H_2CO_3(CO_2 + H_2O)$	62.03				known in soln only
Carbonyl						
chloride	COCl ₂	98.92	1.392	-127.8	7.6	hyd aq; s bz
fluoride	COF ₂	66.01	1.139^{-114}	-114.0	-83.3	hyd aq
sulfide	COS	60.07	1.073°	-138.81	-50.23	54 ²⁰ mL aq; s alc, CS ₂
			$g \cdot L^{-1}$			
Cerium						
(III) chloride	CeCl ₃	246.48	3.92	8.7	1730	100 ²⁰ aq; 30 alc; s acet
(IV) fluoride	CeF ₄	216.12	4.80	>650	d>550	i aq; s a
(IV) oxide	CeO_2	172.13				i aq; s a
(IV) sulfate	Ce(SO ₄) ₂	332.24	3.91	d 195		hyd aq; s H ₂ SO ₄
Cesium						
bromide	CsBr	212.81	4.44	635	1300	107 ¹⁸ aq
carbonate	Cs ₂ CO ₃	325.82		d 610		260 ¹⁵ aq; 11 ²⁰ alc; s eth
chloride	CsCl	168.36	3.988	645	1324	187 ²⁰ aq; 34 ²⁵ MeOH; v s alc
fluoride	CsF	151.90	4.115	703	1231	322 ¹⁸ aq
hydroxide	CsOH	149.91	3.675	272	990	386 ¹⁵ aq; s alc
iodide	CsI	259.81	4.510	621	ca 1280	77 ²⁰ aq; s EtOH; i acet
nitrate	CsNO ₃	194.91	3.685_4^{20}	414	d 849	23 ²⁰ aq; s acet; v sl s alc
oxalate	$Cs_2C_2O_4$	353.82	3.230^{15}			313 aq
selenate	Cs ₂ SeO ₄	408.77	4.4528_4^{20}			244 ¹² aq
sulfate	Cs_2SO_4	361.87	4.243	1019		179 ²⁰ aq; i alc, acet, pyr
Chlorine						
fluoride, tri-	CIF ₃	92.45	1.82511	-76.28	11.74	hyd viol aq; glass wool and org matter ign
(di-) oxide	Cl ₂ O	86.91	3.02^{2}	-120.6	2.1	3.5^{20} aq (hyd to HClO); s CCl ₄
oxide, di-	ClO ₂	67.46	1.642^{0}	-59.6	10.9	11.2 ¹⁰ aq
(di-) oxide, hepta-	Cl_2O_7	182.90	1.805^{25}	-91.5	83.6	d aq; expl on concussion or contact with flame or I ₂
Chlorosulfonic acid Chromium	HSO ₃ Cl	116.52	1.753_4^{20}	-80	158	d viol aq to $HCl + H_2SO_4$
(II) acetate	$Cr(C_2H_3O_2)_2$	170.10				sl s aq, alc; i eth
carbonyl, hexa-	Cr(CO) ₆	220.06	1.77^{18}	d 130	expl 210	i aq, alc, eth

TABLE 2.1 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Chromium						
(II) chloride	CrCl ₂	122.90	2.878	815	1300	v s aq
(III) chloride	CrCl ₃	158.35	2.76^{15}	877	subl 947	i aq, alc, acet, eth
(III) fluoride	CrF ₃	108.99	3.8	1100	subl	i aq, alc; s HF
(III) nitrate 9-water	Cr(NO ₃) ₃ •9H ₂ O	400.15		60	d 100	208 ¹⁵ aq; s alc
(III) oxide	Cr ₂ O ₃	152.02	5.21	2330	3000	i aq, alc
(IV) oxide	CrO ₂	83.99	4.89	$-O_2,300$		i aq; s HNO ₃
(VI) oxide	CrO ₃	99.99	2.70	198	d 250	167 ²⁰ aq; may ign org materials
(III) phosphate 6-water	CrPO ₄ •6H ₂ O	255.06	2.12114	100		i aq; v s a, alk; sl s HOAc
(II) sulfate 7-water	CrSO ₄ ·7H ₂ O	274.17				23 ⁰ aq
(III) sulfate 18-water	Cr ₂ (SO ₄) ₃ •18H ₂ O	716.45	1.7	d 100		220 ²⁰ aq
Chromyl						_
chloride	CrO ₂ Cl ₂	154.90	1.92	-96.5	117	d aq; s eth
Cobalt						
(II) acetate 4-water	$Co(C_2H_3O_2)_2\cdot 4H_2O$	249.08	1.70519	$-4H_2O, 140$		s aq; 2.1 ¹⁵ MeOH
(III) acetate	$Co(C_2H_3O_2)_3$	236.07		d 100		s aq, alc, HOAc
(II) bromide	CoBr ₂	218.75	4.909_4^{25}	678 (in N ₂)		112 ²⁰ aq
(II) carbonate	CoCO ₃	118.94	4.13	d		0.18 ¹⁵ aq; s a
(II) chloride	CoCl ₂	129.84	3.356	740	1087	53 ²⁰ aq
(II) fluoride	CoF ₂	96.93	4.46	1127	1739	1.36 ²⁰ aq; s a
(III) fluoride	CoF ₃	115.93	3.88			d aq; i alc, bz, eth
(II) hydroxide	Co(OH) ₂	92.95	3.597_4^{15}	d		0.0018 aq; s a
(II) iodide	CoI ₂	312.74	5.68	505 d	570 (vac)	203 aq
(II) nitrate 6-water	Co(NO ₃) ₂ •6H ₂ O	291.04	1.87	55	d 74	155 ³⁰ aq; v s alc
(II) oxalate	CoC ₂ O ₄	146.95	3.021_4^{25}	d 250		0.002 ¹⁸ aq; s a
(II) oxide	CoO	74.93	6.45	1805		i aq; s a

(II,III) oxide	Co ₃ O ₄	240.80	6.07	d 900		i aq; v sl s a
(II) sulfate 7-water	CoSO ₄ •7H ₂ O	281.10	2.03_4^{25}	96.8	$-7H_2O, 420$	65 ²⁰ aq; sl s alc
Copper						
(II) acetate hydrate	$Cu(C_2H_3O_2)_2 \cdot H_2O$	199.65	1.882	115	d 240	8 aq; 0.48 MeOH; sl s eth, glyc
(II) acetate-metaarsenite	Cu(C ₂ H ₃ O ₂) ₂ •3Cu-	1013.77				i aq; s a, NH ₄ OH
	$(AsO_2)_2$					
(I) bromide	CuBr	143.45	4.98	488	1318	v sl s aq; s a
(II) bromide	CuBr ₂	223.31	4.710_4^{20}	498		126 aq; s alc, acet, pyr; i bz, eth
(II) chlorate 6-water	Cu(ClO ₃) ₂ •6H ₂ O	338.53		65	d 100	242 ¹⁸ aq; v s alc; s acet
(I) chloride	CuCl	98.99	4.14	430	1212	0.024 aq; s HCl
(II) chloride	CuCl ₂	134.44	3.386_4^{25}	d 300		73 ²⁰ aq; s alc, acet
(II) chloride 2-water	CuCl ₂ ·2H ₂ O	170.47	2.54	$-2H_2O, 100$	d	76 ²⁵ aq; v s alc; s acet
(I) cyanide	CuCN	89.56	2.92	473 (in N ₂)	d	0.00026 aq; s HCl, KCN
(II) fluoride	CuF ₂	101.54	4.23	770	1449	0.075 aq; s a
formate	Cu(OOCH) ₂	153.55	1.831			12.5 aq
hydroxide	Cu(OH) ₂	97.55	3.368	160		i aq; s a
(I) iodide	CuI	190.44	5.62	588	1207	i aq; s HCl, KI
(II) nitrate 3-water	Cu(NO ₃) ₂ •3H ₂ O	241.60	2.05	114.5	d 170	138° aq; v s alc
(II) oleate	Cu(OOCC ₁₇ H ₃₃) ₂	626.43				i aq; sl s alc; s eth
(I) oxide	Cu ₂ O	143.08	6.0	1236	$-O_2$, 1800	i aq; s HCl
(II) oxide	CuO	79.54	6.315_4^{14}	d 1122	-	i aq, alc; s a
(II) perchlorate	Cu(ClO ₄) ₂	262.43	2.225^{23}	82.3	d 130	146^{30} aq; s eth; i bz, CCl ₄
(II) stearate	Cu(OOCC ₁₇ H ₃₅) ₂	630.46		ca 250		i aq, alc, eth; s pyr, hot bz
(II) sulfate	CuSO ₄	159.61	3.603	805 d		14.3° aq
(II) sulfate 5-water	CuSO ₄ ·5H ₂ O	249.68	2.284_4^{16}	$-5H_2O$, 150		32 ²⁰ aq; s MeOH, glyc; sl s EtOH
Cyanogen	NC—CN	52.04	$2.335\mathrm{g}\cdot\mathrm{L}^{-1}$	-27.84	-21.15	420 ²⁰ mL aq; 230 mL alc
azide	NC-N ₃	68.04		detonates		s acetonitrile; can be handled
	_					safely only in solv
bromide	CNBr	105.93	2.015_4^{20}	51.4	61.35	v s aq, alc, eth
chloride	CNCI	61.48	1.186	-6.90	13.0	s aq, alc, eth
iodide	CNI	152.92		146-147	subl 140	s aq, alc, eth
Deuterium	D_2 or 2H_2	4.03	0.169 ^{mp} (lq)	-252.89	-248.24	sl s aq
oxide	D ₂ O or ² H ₂ O	20.03	1.1056^{20}	3.82	101.43	misc aq
	, -			1	'	*

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Disulfuryl dichloride	S ₂ O ₅ Cl ₂	215.03	1.81811	-37.5	152.5	d aq, a
Diphosphoric(V) acid	$H_4P_2O_7$	117.98		61		s aq
Fluorine	F_2	38.00	$1.554^{25}\mathrm{g}\cdot\mathrm{L}^{-1}$	-219.70	-188.20	d aq viol
Fluoroboric acid	HBF_4	87.81		d 130		v s aq
Fluorosulfonic acid	HSO₃F	100.07	1.74315	-87.3	165.5	s aq
-d or [2H]	DSO ₃ F or ² HSO ₃ F	101.08		-89	163	s aq
Germane	GeH ₄	76.62	1.523^{-142}	-165.9	-88.5	sl s hot HCl
Gold						
(III) chloride	AuCl ₃	303.33	3.9	254 d	subl 265	68 ²⁰ aq
Helium	Не	4.00	0.1784 ⁰ g·L ⁻¹ 0.1249 (lq)	-272.2 ^{25 atm}	-268.935	0.861 ²⁰ mL aq
Hydrazine	H ₂ NNH ₂	32.05	1.0083^{20}	1.54	113.8	misc aq, alc
hydrate	H ₂ NNH ₂ ·H ₂ O	50.16	1.038^{21}	-51.7	119.4	misc aq, alc
Hydrazinium						1,
(1+) chloride	H ₂ NNH ₃ Cl	68.51		92.6	d 240	v s aq
(2+) chloride	ClH ₃ NH ₃ Cl	104.97	1.4226^{20}	198	d 200	v s ag; sl s alc
(2+) sulfate	(H ₃ NNH ₃)SO ₄	130.13	1.378	254	d	3.4 ²⁰ aq; i alc
Hydrogen	H_2	2.02	$0.0899\mathrm{g}\cdot\mathrm{L}^{-1}$	-259.76	-252.76	1.9 mL aq
azide	HN_3	43.03	1.126	-80	37	v s aq (v expl)
borate (1-)	HBO_2	43.83	2.486	236		v sl s aq
borate $(3-)$, ortho-	H_3BO_3	61.83	1.435^{15}	171.0	d 300	6.4 ³⁰ aq
bromide	HBr	80.92	$3.388^{20} \mathrm{g} \cdot \mathrm{L}^{-1}$ $2.160^{-66} \mathrm{(lq)}$	-86.81	-66.71	193 ²⁵ aq; s alc
bromide	$48\% HBr + H_2O$		1.49 g • L-1	-11	126	v s aq (constant boiling)
bromide-d	DBr or ² HBr	81.92	$3.39^{20}\mathrm{g}\cdot\mathrm{L}^{-1}$	-87.46	-66.5	v s aq

chloride	HC1	36.46	1.526 ²⁰ g·L ⁻¹	-114.18	-85.00	72 ²⁰ aq
chloride	20.24% HCl + H ₂ O		1.187 ⁻⁸⁵ (lq) 1.097		110	v s aq (constant boiling)
cyanide	HCN	27.06	0.901 g·L ⁻¹	-13.24	25.70	v s aq (constant bonnig)
Cyanide	HCN	27.00		-13.24	23.70	v s aq
fluoride	HF	20.01	1.2675 ¹⁰ (lq) 0.922 ⁰ g • L ⁻¹	-83.57	19.52	v s aq
			0.957 ¹⁹ (lq)			
fluoride	35.35% HF + H ₂ O		(14)		120	v s aq (constant boiling)
iodide	HI	127.92	5.37 ²⁰ g·L ⁻¹	-50.79	-35.35	70° aq
			2.799^{-35} (lg)			
iodide	57% HI + H ₂ O		1.70 ¹⁵		127	v s aq (constant boiling)
nitrate	HNO ₃	63.02	1.5027	-41.59	83	v s aq
nitrate	69% HNO ₃ + H ₂ O		1.41^{20}		120.5	misc aq (constant boiling)
oxide	H ₂ O	18.02	1.000^4	0.00	100.00	
oxide- d_2	D ₂ O or ² H ₂ O	20.03	1.1045	3.82	101.43	misc aq
perchlorate 2-water	HClO₄•2H ₂ O	136.49	1.67^{20}	-17.8	203	v s aq (commercial 72% a)
periodate(1-)	HIO ₄	191.91		subl 110	d 138	440 ²⁵ aq
periodate(5-)	H ₅ IO ₆	227.94		130	d 140	113 ag
peroxide	H_2O_2	34.02	1.4649^{0}	-0.40	151.2	misc aq; s alc, eth
phosphate(V) $(1-)$	HPO ₃	79.98	2.2-2.5	subl		s aq
phosphate(V) $(3-)$	H ₃ PO ₄	98.00	1.88	42.3	d 213	v s aq (commercial 85% a)
phosphide	PH ₃	34.00	1.529	-133.81	-87.78	26 ¹⁷ mL aq; s alc, eth
			g•L ⁻¹			
selenide	H ₂ Se	80.98	2.12^{-42}	-65.73	-42	9.5 ²⁰ mL aq
sulfide	H ₂ S	34.08	1.1906	-85.52	-60.33	0.334 ²⁵ mL aq
			$g \cdot L^{-1}$			
telluride	H ₂ Te	129.63	6.234	-49	-2	d aq
			$g \cdot L^{-1}$			
tungstate(VI) (2-)	H_2WO_4	249.86	5.5	$-H_2O, 100$		i aq; s alk, HF
Hydroxylamine	HONH ₂	33.03	1.332	33.1	58 ^{22 mm}	s aq, alc
Hydroxylammonium						
chloride	HONH ₃ Cl	69.49	1.680^{20}	150.5	d	83 ¹⁷ aq; 4.4 ²⁰ alc
sulfate	(HONH ₃) ₂ SO ₄	164.14		d 170		69 ²⁰ aq
	I	ı	1	1	ı	1

 TABLE 2.1
 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Iodic acid	HIO ₃	175.91	4.6290	d 110 to H ₅ IO ₆	d 195 to I ₂ O ₅	310 ¹⁶ aq
Iodine	I_2	53.82	4.660^{20}	113.60	184.24	0.029 ²⁰ aq; s alc, bz, chl, CS ₂ , CCl ₄ , eth
bromide	IBr	206.81	4.4157^{0}	42	116.d	s aq, alc, eth
chloride	ICl	162.36	3.20	27.38	97.8	d aq; s alc, eth
chloride, tri-	ICl ₃	233.26	3.202	101 d		d aq; s alc, bz, eth
fluoride, penta-	IF ₅	221.90	3.252	8.5	102	d aq
fluoride, hepta-	IF ₇	259.89	$2.8^6\mathrm{g}\cdot\mathrm{L}^{-1}$	4.5	5.5	
(di-) oxide, penta-	I_2O_5	333.81	4.799^{25}	d 275		187 ¹³ aq
Iron	Fe	55.85	7.86	1537	2872	i aq; s a
(II) bromide	FeBr ₂	215.67	4.636	691	934	117 ²⁰ aq
(III) bromide	FeBr ₃	295.57		subl		s aq
carbonyl, penta-	Fe(CO) ₅	195.00	1.49	-21	103	i aq; s alc, bz, eth
(II) chloride	FeCl ₂	126.75	3.16^{25}	677	1024	63 ²⁰ aq; v s alc, acet;i eth
(III) chloride	FeCl ₃	162.21	2.898	304	332	74º aq
(III) ferrate(II),	$Fe_4[Fe(CN)_6]_3$	859.25	1.80	d		i aq; s HCl
hexacyano-						
(II) fluoride	FeF ₂	93.84	4.09	1100	1837	sl s aq; s a
(III) fluoride	FeF ₃	112.84	3.87	subl 927		0.091 ²⁵ aq; s a; i alc, bz
(II) iodide	FeI_2	309.66	5.315	587	1093	s aq
(III) nitrate 9-water	$Fe(NO_3)_3 \cdot 9H_2O$	404.02	1.684^{21}	47	d 100	138^{20}
(II) oxalate 2-water	$FeC_2O_4 \cdot 2H_2O$	179.90	2.28	d 150–160		0.044 ¹⁸ aq; s a
(II) oxide	FeO	71.85	5.7	1377	d 3414	i aq; s a
(III) oxide	Fe_2O_3	159.69	5.24	1462 d		i aq; s HCl
(II, III) oxide	Fe ₃ O ₄	231.54	5.1	1597		i aq; s a
(II) sulfate 7-water	FeSO ₄ •7H ₂ O	278.04	1.89			48^{20} aq

(III) sulfate	Fe ₂ (SO ₄) ₂	399.88	3.09718	d 1178		sl s aq (hyd); sl s alc
(III) sulfate 9-water	$Fe_2(SO_4)_3 \cdot 9H_2O$	562.01	2.1	d 175		440 aq
Krypton	Kr	83.80	3.736	-157.2	-153.4	5.94 ²⁰ mL aq
			g • L ⁻¹			_
Lead	Pb	207.21	11.34 (fcc)	327.50	1753	i aq; s HNO ₃
(II) acetate 3-water	$Pb(C_2H_3O_2)_2 \cdot 3H_2O$	379.33	2.55	d 200		46 ¹⁵ aq
(IV) acetate	$Pb(C_2H_3O_2)_4$	443.37	2.228^{17}	175		d aq; s chl
(II) azide	$Pb(N_3)_2$	291.23		expl 350		0.023 ¹⁸ aq; s HOAc
(II) carbonate	PbCO ₃	267.20	6.6	d 340		i aq; s a, alk
(II) chromate(VI) (2-)	PbCrO ₄	323.18	6.1215	844	d	i aq; s a
(IV) fluoride	PbF ₄	283.21	6.7	600		hyd aq
(II) nitrate	Pb(NO ₃) ₂	331.23	4.53^{20}	d 200		56 ²⁰ aq; 1.3 MeOH
(II) oleate	$Pb(C_{18}H_{33}O_2)_2$	770.12				i aq; s alc, bz, eth
(II) oxide	PbO	223.21	9.53	886	1516	0.0017^{20} ; s HNO ₃
(IV) oxide	PbO ₂	239.21	9.375	d 752		i aq; s HCl
(II) phosphate	$Pb_3(PO_4)_2$	811.59	6.9	1014		i aq; s HNO ₃ , alk
(II) stearate	$Pb(C_{18}H_{35}O_2)_2$	774.15		ca 125		0.05^{35} aq; s hot alc
(II) sulfate	PbSO ₄	303.28	6.2	1090		0.004 aq
Lithium	Li	6.94	0.535^{20}	180.6	1340	d aq to LiOH
aluminate, tetrahydrido-	LiAlH ₄	37.95	0.917	d 125		d aq, alc; 30 eth (flammable)
amide	LiNH ₂	22.96	1.17818	374	d 430	d aq; i bz, eth
benzoate	LiC ₇ H ₅ O ₂	128.05		>300		33 aq; 7.7 alc
boronate	LiBH ₄	21.79	0.666	268	d 380	d aq; s eth, THF
bromate	LiBrO ₃	134.85	3.62			179 ²⁰ aq
bromide	LiBr	86.84	3.464	550	1289	164 aq; s alc, eth
carbonate	Li ₂ CO ₃	73.89	2.11^{0}	720	d	1.3 ²⁰ aq; i alc; s a
chloride	LiCl	42.40	2.068	610	1383	77 ²⁰ aq; s alc, acet
fluoride	LiF	25.94	2.640^{20}	846	1717	0.13 ²⁵ aq; s a
hydride	LiH	7.95	0.780	688.7	d 950	d aq; no known solv (flammable)
hydroxide	LiOH	23.95	2.54	471.2	1626	12.4 ²⁰ aq
iodide	LiI	133.84	4.061	467	1178	165 ²⁰ aq; v s alc
iodide 3-water	LiI·3H ₂ O	187.89	3.5	73	$-3H_2O, 300$	200 aq; 200 alc
nitrate	LiNO ₃	68.94	2.38	261	-	70 ²⁰ aq; s alc

TABLE 2.1 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Lithium						
perchlorate	LiClO ₄	106.40	2.43^{25}	236	d 400	56 ²⁰ aq
sulfate	Li ₂ SO ₄	109.88	2.22	860		34.5 ²⁰ aq
Magnesium	Mg	24.31	1.74^{20}	650	1105	i aq; s a
amide	$Mg(NH_2)_2$	56.37	1.39_4^{25}	ign in air		d viol aq giving NH ₃
bromide	$MgBr_2$	184.13	3.72	711	1158	101 ²⁰ aq
bromide 6-water	MgBr ₂ ·6H ₂ O	292.22	2.00	165 d		160 ²⁰ aq; s alc
carbonate	MgCO ₃	84.32	2.958	d 402		0.01 aq; s a
chloride	MgCl ₂	95.23	2.41	714	1437	54.6 ²⁰ aq
hydride	MgH_2	26.34	1.45	d 287 (vac)	ign air	d viol aq, alc
hydroxide	Mg(OH) ₂	58.33	2.36	268 d		i aq; s a
oleate	$Mg(C_{18}H_{33}O_2)_2$	293.61				i aq; s alc, eth, PE
oxide	MgO	40.52	3.58	2825	3260	i aq; s a
perchlorate	$Mg(ClO_4)_2$	223.23	2.21^{20}	d 251		49.6 aq
sulfate 7-water	MgSO ₄ ·7H ₂ O	246.49	1.67	$-6H_2O, 120$	$-7H_2O, 250$	27.2 aq; s alc
sulfite 6-water	MgSO ₃ ·6H ₂ O	212.47	1.725	$-6H_2O, 200$	d	66 ²⁵ aq
Manganese						
acetate 4-water	$Mn(C_2H_3O_2)_2 \cdot 4H_2O$	245.08	1.589			38 ⁵⁰ aq; s alc
bromide 4-water	$MnBr_2 \cdot 4H_2O$	286.82		54d		200 aq; s alc
carbonate	MnCO ₃	114.94	3.125	d		0.0065 ²⁵ aq; s a
(di-) carbonyl, deca-	$Mn_2(CO)_{10}$	389.99	1.75^{25}	155 (CO atm)	d 110	i aq; s org solv
chloride 4-water	MnCl ₂ ·4H ₂ O	197.91	2.01	$-4H_2O, 198$		143 aq; s alc; i eth
(III) fluoride	MnF ₃	111.93	3.54	d 600		hyd aq; s a
nitrate 6-water	$Mn(NO_3)_2 \cdot 6H_2O$	287.05	1.8	25.8		v s aq, alc
(IV) oxide	MnO_2	86.94	5.026	d 530		i aq; s HCl
sulfate hydrate	MnSO ₄ ·H ₂ O	169.01	2.95	$-H_2O, 400$		$70^{20} \mathrm{aq}$

Mercury	Hg	200.59	13.59420	-38.86	356.60	i aq; s HNO ₃
(II) acetate	$Hg(C_2H_3O_2)_2$	318.70	3.28	178		25 ¹⁰ aq; 7.5 ¹⁵ MeOH
(II) bromide	HgBr ₂	360.44	6.05	241	subl > 241	0.56^{20} aq; 20^{25} alc
(I) chloride	Hg ₂ Cl ₂	472.09	7.150	subl 382	d	0.00027 aq; s aqua regia
(II) chloride	HgCl ₂	271.52	5.44	277	304	6.6 ²⁰ aq; 33 alc; 4 eth
(II) cyanide	Hg(CN) ₂	252.65	3.996	d 320		9.3 ²⁰ aq; 8 alc; 25 MeOH
(II) fluoride	HgF ₂	238.61	8.9515	645	647	hyd aq; s HF
(II) iodide	Hgl ₂	454.45	6.28	259	350	0.006 ²⁵ aq; 1 alc; 1.7 acet
(II) nitrate	Hg(NO ₃) ₂	324.63	4.3	79	d	v s aq; s acet
(II) oxide	HgO	216.61	11.14	d 476		0.005 ²⁵ aq; s a
(I) sulfate	Hg_2SO_4	497.29	7.56	d		0.06^{25} aq; s HNO ₃
(II) sulfate	HgSO ₄	296.68	6.47	d		d aq; s a
(II) sulfide, red	HgS	232.68	8.10	subl 583		i aq; s aqua regia
Molybdenum						
carbonyl, hexa-	Mo(CO) ₆	264.02	1.96	subl 102	156.4	s bz
(V) chloride	MoCl ₅	273.21	2.928	194	264	hyd aq; s conc a
(VI) oxide	MoO ₃	143.95	4.696^{26}	801	1155	0.22 ²⁸ aq; s alk, NH ₃
sulfide, di-	MoS ₂	160.08	5.06^{15}	2375	subl 450	i aq; s aqua regia
Molybdic acid hydrate	H ₂ MoO ₄ ·H ₂ O	179.97	3.124^{15}	$-H_2O, 70$		0.133 ¹⁸ ; s alk
Molybdic phosphoric	$H_7[P(Mo_2O_7)_6] \cdot 28H_2O$	2365.71	2.53	78		hyd aq
acid						
Neon	Ne	20.18	$0.8899^{0}\mathrm{g}\cdot\mathrm{L}^{-1}$	-248.6	-246.1	1.05^{20}mL aq
Nickel	Ni	58.71	8.90	1455	2920	i aq; s HNO ₃
acetylacetonate	$Ni(C_5H_7O_2)_2$	256.93	1.455^{17}	229	235	s aq, alc, bz, chl
bromide	NiBr ₂	218.53	5.098	963	subl	131 ²⁰ aq
chloride 6-water	NiCl ₂ ·6H ₂ O	237.70				111 ²⁰ aq
dimethylglyoxime	$Ni(HC_2H_6N_2O_2)_2$	288.91		subl 250		i aq; s abs alc, a
formate 2-water	Ni(OOCH) ₂ ·2H ₂ O	184.78	2.154^{20}	$-2H_2O$, 130	d 180	s aq; i alc
nitrate 6-water	$Ni(NO_3)_2 \cdot 6H_2O$	290.81	2.05	56.7	136.7	150 ²⁰ aq
sulfate 6-water	NiSO ₄ ·6H ₂ O	262.86	2.07	53.3		$40^{20} \mathrm{aq}$

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Niobium						
(V) chloride	NbCl ₅	270.20	2.75	204	250	s HCl, CCl₄
(V) fluoride	NbF ₅	187.91	2.70_4^{80}	80	235	hyd aq, alc
(V) oxide	Nb_2O_5	265.82	4.6	1512		i aq; s HF, hot H ₂ SO ₄
Nitrogen	N_2	28.01	1.165^{20}	-210.00	-195.81	$1.52^{20}\mathrm{mL}$ aq
			$g \cdot L^{-1}$			•
[15N]	$^{15}N_2$	30.01	1.25^{20}	-209.95	-195.73	
			$g \cdot L^{-1}$			
chloride, tri-	NCl ₃	120.37	1.653^{20}	-27	71	i aq; s bz, CS ₂ , CCl ₄
(di-) oxide	N_2O	44.02	1.8433^{20}	-90.85	-88.47	1300 mL aq; s alc
			$g \cdot L^{-1}$			
oxide	NO	30.01	1.2488^{20}	-163.64	-151.76	7º mL aq
			$g \cdot L^{-1}$			
(di-) oxide, tetra-	N_2O_4	92.02	1.447_4^{20}	-9.3	21.10 d	d aq; s HNO ₃ , H ₂ SO ₄ , chl
(di-) oxide, penta-	N_2O_5	108.01	2.05^{15}	30	47.0	s aq, chl
Nitrosyl						
chloride	NOCl	65.47	1.592^{-5}	-61.5	-5.5	hyd aq
fluoride	NOF	49.01	2.788^{20}	-132.5	-59.9	hyd aq
			$g \cdot L^{-1}$			
Nitryl						
chloride	NO ₂ Cl	81.46	2.81^{100}	-145	-13.5	d aq
			$g \cdot L^{-1}$			
fluoride	NO_2F	65.00	2.7^{20}	-166.0	-72.4	d aq
			$g \cdot L^{-1}$			
Osmium oxide, tetra-	OsO_4	254.20	4.91	40.6	130.0	7.24 ²⁵ aq; 375 ²⁵ CCl ₄
Oxygen	O_2	32.00	1.331^{20}	-218.75	-182.96	36 ²⁵ mL aq
			$g \cdot L^{-1}$			

Ozone	O_3	48.00	1.99820	-192.5	-110.50	49.4^0 mL aq
D II II	D.1	106.4	g·L ⁻¹	1550	20.40	1 JUNIO IL GO
Palladium	Pd	106.4	12.023	1550	2940	s hot HNO ₃ , H ₂ SO ₄
acetate	$Pd(C_2H_3O_2)_2$	224.49	- 10	205d		i aq, alc; s acet, chl
chloride	PdCl ₂	177.30	4.0^{18}	680	d 680	s aq
nitrate	$Pd(NO_3)_2$	230.42		d		hyd aq; s HNO ₃
oxide	PdO	122.40	8.70^{20}	870 d		i aq, a
Perchloryl fluoride	ClO ₃ F	102.46	0.637	-147.74	-46.67	
Phosphine	PH_3	34.00	1.529	-133.81	-87.78	26 ¹⁷ mL aq; s alc, eth
			$g \cdot L^{-1}$			
Phosphinic acid	HPH_2O_2	66.00	1.49319	26.5	d 50	s aq
Phosphonic acid	H_2PHO_3	82.00	1.651^{21}	ca 73	d 180	v s aq, alc
Phosphoric acid						
meta-	HPO ₃	79.98	2.2-2.5			slowly hyd aq; s alc
ortho-	H_3PO_4	98.00	1.88	42.35		
commercial 85% acid			1.685	anhyd 150	to $H_4P_2O_7$	v s aq
					ca 200; to	
					$HPO_3 > 300$	
fluoro-	H ₂ PO ₃ F	99.99	1.818	-80		
Phosphorus						
(white)	P (P ₄ molecules)	30.97	1.828	44.2	280.3	i aq; 0.025 alc; 1 eth; 2.5 chl, bz; 1.25 CS ₂
(red)	P	30.97	2.34	597	subl 416	i aq (ign in air 260°C)
bromide, tri-	PBr ₃	270.73	2.8515	-40.5	173.2	d aq, alc; s acet, CS ₂
bromide, penta-	PBr ₅	430.56	3.46^{20}	d 100		d aq; s CCl ₄ , CS ₂
chloride, tri-	PCl ₃	137.35	1.575^{20}	-91	75	d aq, alc; s bz, chl
chloride, penta-	PCl ₅	208.27	2.119^{20}	subl 100	166 d	hyd ag; s CCl ₄ , CS ₂
fluoride, penta-	PF ₅	125.98	5.805	-93.8	-84.6	hyd aq
, _F	3		$g \cdot L^{-1}$	1000		,
(tetra-) oxide, hexa-	P_4O_4	219.90	2.136_4^{20}	24	$175 (in N_2)$	hyd aq; s bz, CS ₂
(tetra-) oxide, deca-	P_4O_{10}	283.88	2.30	340	subl 360	d aq; s H ₂ SO ₄
(tetra-) selenide, tri-	P ₄ Se ₃	360.80	1.31	245	360–400	hyd ag; s bz, chl, acet
(tetra-) sulfide, deca-	P_4S_{10}	444.54	2.09	288	514	hyd aq; s alk, CS ₂

 TABLE 2.1
 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Phosphoryl chloride, tri-	POCl ₃	153.35	1.645 ²⁵	2	105	d aq, alc
Platinic(IV) acid	$H_2PtCl_6 \cdot 6H_2O$	517.92	2.431	60		v s aq, alc
6-water, hexachloro-						_
Platinum	Pt	195.09	21.45^{20}	1770	3824	i aq; s aqua regia, fused alk
Platinum						
(II) chloride	PtCl ₂	266.00	6.05	d 581		i aq; s HCl, NH ₄ OH
(IV) oxide	PtO ₂	227.09	10.2	450		i aq, aqua regia
Potassium	K	39.10	0.856^{20}	63.7	765.5	d to KOH aq; s a
acetate	$KC_2H_3O_2$	98.14	1.57^{25}	292		256 ²⁰ aq; 34 alc
bismuthate(4—),	K_4BiI_7	1253.82				d aq; s alk iodide soln
heptaiodo-						
borate, tetrahydrido-	KBH_4	53.95	1.11	d 497		21 ²⁵ aq; 3.5 ²⁰ MeOH
bromate	KBrO ₃	167.01	3.27^{17}	350	d 370	6.9 ²⁰ aq
bromide	KBr	119.01	2.75	734	1398	65 ²⁰ aq; 0.4 alc
carbonate	K ₂ CO ₃	138.20	2.29	901	d	111 ²⁰ aq; i alc
chlorate	KClO ₃	122.55	2.238^{20}	368	d 368	7.3 ²⁰ aq; 2 glyc
chloride	KC1	74.56	1.988	771	1437	34 ²⁰ aq; 7 glyc
chromate(VI)	K ₂ CrO ₄	194.20	2.732^{18}	975		64 ²⁰ aq; i alc
citrate hydrate	$K_3C_6H_5O_7 \cdot H_2O$	324.42	1.98	d 230		167 ¹⁵ aq
cobaltate(III) 1.5-water,	$K_3[Co(NO_2)_6] \cdot 1.5H_2O$	479.30		d 200		0.089 ¹⁷ aq; v sl s alc
hexanitrito-						
cyanate	KOCN	81.11	2.048	d 700–900		s aq; sl s alc
cyanide	KCN	65.12	1.52^{16}	622	1625	50 aq
dichromate(VI)	$K_2Cr_2O_7$	294.19	2.676^{25}	398	d 500	12.3 ²⁰ aq
disulfate(IV)	$K_2S_2O_5$	222.32				s aq (flammable if ground)

ethyldithiocarbonate	KC ₂ H ₅ OCSS	160.30	1.55822	d 200		v s aq
ferrate(III), hexacyano-	K ₃ [Fe(CN) ₆]	329.26	1.89	d		84 ²⁰ aq (slow)
fluoride	KF	58.10	2.481	858	1517	95 ²⁰ aq
formate	KOOCH	84.10	1.91	167.5	d 168	337 ²⁰ aq
gluconate	KC ₆ H ₁₁ O ₇	234.24		d 180		v s aq; i alc, bz, chl
hydride	KH	40.11	1.43	417 d		d aq
hydrogen arsenate, di-	KH ₂ AsO ₄	180.02	2.867	288		19 ⁶ aq; 63 gly; i alc
hydrogen carbonate	KHCO ₃	100.11	2.17	d 100-200		34 ²⁰ aq
hydrogen difluoride	KHF ₂	78.11	2.37	238.7	d 478	30 ²⁰ aq; s alc
hydrogen bisiodate	KH(IO ₃) ₂	389.92				1.3 ¹⁵ aq
hydrogen oxalate	KHC ₂ O ₄	128.11	2.044	d		2.5 aq
hydrogen bisoxalate	$KH_3(C_2O_4)_2 \cdot 2H_2O$	254.20	1.836	d		1.8 ¹³ aq
dihydrate, tri-						
hydrogen phosphate	K ₂ HPO ₄	174.18		d		150 aq
hydrogen phosphate, di-	KH ₂ PO ₄	136.09	2.338	400	d	22.6 ²⁰ aq
hydrogen phthalate	KHC ₈ H ₄ O ₄	204.22	1.636 ²⁵	d		10.2 aq; sl s alc
hydrogen sulfate	KHSO ₄	136.17	2.24	197	d	48 ²⁰ aq
hydrogen tartrate	KHC ₄ H ₄ O ₆	188.18	1.956			0.5 ²⁰ aq
hydroxide	KOH	56.11	2.044	406	1320	112 ²⁰ aq; 33 alc
iodate	KIO ₃	214.02	3.89^{25}	560 d		8.1 ²⁰ aq; i alc
iodide	KI	166.02	3.12	681	1345	144 ²⁰ aq; 4,5 alc; 1.2 acet
manganate(VI)	K ₂ MnO ₄	197.12		d 190		s aq (stable in KOH)
nitrate	KNO ₃	101.10	2.109^{16}	334.3	d 400	32 ²⁰ aq; 0.16 alc; s glyc
nitrite	KNO ₂	85.10	1.915	441	d 250	306 ²⁰ aq
oxalate hydrate	$K_2C_2O_4 \cdot H_2O$	184.24	2.127^4	$-H_2O$, 160	d	36 ²⁰ aq
periodate	KIO ₄	230.01	3.618_4^{15}	582 d		0.42 ²⁰ aq
permanganate	KMnO ₄	158.03	2.703	d 240		6.34 ²⁰ aq
peroxide	K_2O_2	110.20		490		d
peroxodisulfate	$K_2S_2O_8$	270.32	2.477	d 100		5.3 ²⁰ aq
phenolsulfonate hydrate	KC ₆ H ₄ (OH)SO ₃ ·H ₂ O	240.28	1.87			s aq, alc
phosphate	K_3PO_4	212.28	2.56417	1340		92 ²⁰ aq
selenocyanate	KSeCN	144.08		d 100		s aq
	I	ı	1	1	1	ı

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Potassium						
silicate(2-)	K ₂ SiO ₃	154.29		976		s aq
silicate, hexafluoro-	K ₂ SiF ₆	220.25	2.27	d		sl s aq
sodium tartrate 4-water	KNaC ₄ H ₄ O ₆ ·4H ₂ O	282.23	1.790	70–80	d 220	54 ¹⁵ aq
sorbate	KC ₆ H ₇ O ₂	150.22	1.363	d 270		110 ²⁰ aq
stannate(IV) 3-water	$K_2SnO_3 \cdot 3H_2O$	298.94	3.197	$-3H_2O, 140$		100 ²⁰ aq
sulfate	K ₂ SO ₄	174.27	2.662	1067	1670	11 ²⁰ aq; 1.3 glyc; i alc
sulfite dihydrate	K ₂ SO ₃ ·2H ₂ O	194.30		d		106 ²⁰ aq
thiocarbonate	K_2CS_2	186.41		d		v s aq
thiocyanate	KSCN	97.18	1.886^{14}	173	d 500	217 ²⁰ aq; 200 acet; 8 alc
						acet; 8 alc
thiosulfate	$K_2S_2O_3$	190.33		d 400		155 ²⁰ aq
titanate(IV), oxobis-	$K_2[TiO(C_2O_4)_2(H_2O)_2]$	354.18				v s aq
(oxalato)diaqua-						
Rhenium(VII) sulfide	Re_2S_7	596.85	4.866	d 460		i aq; s HNO ₃
Rhodium(III) chloride	RhCl ₃	209.28		d 450	subl 850	i aq; s KOH, KCN
Rubidium						
chloride	RbCl	120.94	2.76	715	1381	91 ²⁰ aq; 1.1 MeOH
iodide	RbI	212.37	3.55	640	1304	144 ¹⁸ aq
nitrate	RbNO ₃	147.47	3.11	310		53 ²⁰ aq
sulfate	Rb ₂ SO ₄	267.03	3.613^{20}	1060		48^{20} aq
Ruthenium						
(III) chloride	RuCl ₃	207.47	3.11	d 500		i aq; s HCl, alc
(IV) oxide	RuO_2	133.07	6.97	d		i aq; s fused alk
Selenic acid	H ₂ SeO ₄	144.98	2.9508_4^{15}	58	260	567 ²⁰ aq (viol)
Selenium	Se	78.96	4.81^{20}	221	685	s CS ₂ , KOH, KCN
(IV) oxide	SeO ₂	110.96	3.954_{15}^{15}	340	subl 315	38 ¹⁴ aq; 10 ¹² MeOH

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	(di-) sulfide, hexa-	Se_2S_6	350.28	2.44	121.5		i aq; 1.2 bz; s CS ₂
Silicon Si 28.09 2.33°5 1415 2680 s HF + HNO₃, fused alk oxides s fused alk oxides s fused alk oxides s fused alk oxides s fused alk oxides sothiocyanate, tetra-oxide, di - (quartz) SiCl₄ 40.07 3.217 subl 2700 d 2972 s fused alk oxides and profile and pr	(tetra-) sulfide, tetra-		444.08	3.20	113		i aq; 0.04 bz; s CS ₂
$ \begin{array}{c} \text{carbide} \\ \text{chloride} \\ \text{chloride} \\ \text{chloride} \\ \text{SiCl}_4 \\ \text{siothiocyanate, tetra-} \\ \text{oxide, di- (quartz)} \\ \text{oxide-tungsten} \\ \text{tioxide-water} \\ \text{(1/12/26) (silico-tungste acid)} \\ \text{telluride, tri-} \\ \text{Si}(\text{NCS})_4 \\ \text{SiO}_2 \\ \text{Oxide-tungsten} \\ \text{(1/12/26) (silico-tungste)} \\ \text{telluride, tri-} \\ \text{Si}_2 \\ \text{SiO}_2 \\ \text{SiO}_2 \\ \text{SiO}_2 \\ \text{SiO}_2 \\ \text{2BWO}_3 \cdot 26\text{H}_2\text{O} \\ \text{SiI}_2 \\ \text{Oxide-tungste} \\ \text{Ag} \\ \text{acetate} \\ \text{AgC}_2 \\ \text{H}_3\text{O}_2 \\ \text{Ag} \\ \text{aride} \\ \text{AgN}_3 \\ \text{carbonate} \\ \text{AgCO}_3 \\ \text{chloride} \\ \text{AgCl}_3 \\ \text{chloride} \\ \text{AgCl}_3 \\ \text{chloride} \\ \text{chromate(VI)} \\ \text{Cyanide} \\ \text{AgF}_1 \\ \text{cluride} \\ \text{AgC}_3 \\ \text{cluride} \\ \text{AgC}_3 \\ \text{cluride} \\ \text{AgCN}_3 \\ \text{cluride} \\ \text{AgCN}_3 \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{331.77} \\ \text{5.625}^{235} \\ \text{5.625}^{235} \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{cluride} \\ \text{AgCN}_3 \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{33.177} \\ \text{5.625}^{235} \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{33.177} \\ \text{5.625}^{235} \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{33.177} \\ \text{5.625}^{235} \\ \text{cluride} \\ \text{AgCN}_4 \\ \text{133.90} \\ \text{3.95} \\ \text{5.852}^{16} \\ \text{435} \\ \text{1150} \\ \text{172}^{23} \\ \text{aq} \\ \text{i aq; s KCN} \\ \text{11000ide} \\ \text{AgF}_5 \\ \text{145.87} \\ \text{4.57} \\ \text{690} \\ \text{d} \\ \text{400} \\ \text{d} \\ \text{d} \\ \text{d} \\ \text{0.0002}^{23} \\ \text{aq} \\ \text{i aq; s KCN} \\ \text{litrate} \\ \text{AgNO}_3 \\ \text{i fersion}_4 \\ \text{324.80} \\ \text{5.683}^{30} \\ \text{5.852}^{16} \\ \text{435} \\ \text{1150} \\ \text{1172}^{23} \\ \text{aq} \\ \text{d} \\ $	Silane	SiH ₄	32.09	0.68^{-185}	-184.7	-111.9	d aq slowly
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Silicon	Si	28.09	2.33^{25}	1415	2680	s HF + HNO ₃ , fused alk oxides
isothiocyanate, tetra- oxide, di- (quartz) oxide, tungsten trioxide-water (1/12/26) (silico- tungstic acid) telluride, tri- Silver Ag acetate AgC,H ₂ O ₂ 149.89 252 297 252 297 26.40 331.049 ¹⁵ 390.15 2164 i aq; s HNO ₃ 1.049 ¹⁶ aq acetate AgC,H ₂ O ₂ 166.92 3.259 ¹⁵ d azide AgN ₃ 149.89 carbonate Ag.CO ₃ 275.77 6.077 d.220 chlorate AgClO ₃ 191.34 4.430 ²⁰ 231 d.270 15.3 ²⁰ aq chloride AgCl AgCl AgCl AgCl AgCl 331.77 5.6252 ³⁵ chloride AgCN 133.90 3.95 d 320 fluoride AgCN 133.90 145.87 4.57 690 d 700 d 700 hyd viol aq i aq; s HNO ₃ i aq; s HNO ₃ 1.049 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0003 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0003 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0003 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ (expl) 0.0002 ²⁰ aq i aq; s KCN, HNO ₃ aq i aq; s HN	carbide	SiC	40.07	3.217	subl 2700	d 2972	s fused alk
oxide, di-(quartz) SiO₂ oxide-tungsten trioxide-water (1/12/26) (silicotungstic acid) telluride, tri- SiO₂ · 12WO₃ · 26H₂O 438.97 and a single s	chloride	SiCl ₄	169.89	1.48^{20}	-70	57.6	hyd aq; s bz, CCl ₄ , eth
oxide, di-(quartz) SiO ₂ SiO ₂ · 12WO ₃ · 26H ₂ O 60.08 310.66 2.64-2.66 1423 2230 i aq; s HF vs aq, alc vioxide-tungsten trioxide-water (1/12/26) (silicotungstic acid) telluride, tri- Si, Te ₃ 438.97 892 107.87 10.4915 960.15 2164 i aq; s HNO ₃ 1.04200 aq 1.04200	isothiocyanate, tetra-	Si(NCS) ₄	260.40		143.8	314.2	d aq
oxide-tungsten trioxide-water (1/12/26) (silicotungstic acid) SiQ2-12WO3-26H2O 3310.66 892 Silver Ag actate acide aride carbonate AgCP4, O2 across (horate chorate AgCI and a silicotate agricultural chorate chorate AgCI and a silicotate agricultural chorate chorate agricultural		SiO ₂	60.08	2.64-2.66	1423	2230	1
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			3310.66				-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	trioxide-water	2 3 2					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	(1/12/26) (silico-						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	tungstic acid)						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	telluride, tri-	Si ₂ Te ₃	438.97		892		
azide AgN_3 149.89 252 297 i aq; s KCN, HNO ₃ (expl) carbonate $Ag2CO_3$ 275.77 6.077 d 220 0.003³0 aq chlorate $AgClO_3$ 191.34 4.430²0 231 d 270 15.3²0 aq chloride $AgCl$ 143.34 5.56 455 1564 0.00019 aq; s NH ₄ OH chromate(VI) $Ag2CrO_4$ 331.77 5.625²5 0.002²0 aq; s HNO ₃ , NH ₄ OH cyanide $AgCN$ 133.90 3.95 d 320 i aq; s KCN fluoride AgF 126.88 5.852¹6 435 1150 172²0 aq (II) fluoride AgF_2 145.87 4.57 690 d 700 hyd viol aq iodate $AgIO_3$ 282.80 5.525²0 >200 d 0.004²0 aq iodide AgI 234.80 5.683³0 558 1505 i aq; s KCN nitrate $AgNO_3$ 169.89 4.352¹9 210 d 440 216²0 aq nitrite $AgNO_2$ 153.89 4.453 d 140 0.41²²5 aq 0.	Silver	Ag	107.87	10.49^{15}	960.15	2164	i aq; s HNO ₃
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	acetate	AgC ₂ H ₃ O ₂	166.92	3.259^{15}	d		1.04 ²⁰ aq
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	azide	AgN_3	149.89		252	297	i aq; s KCN, HNO ₃ (expl)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	carbonate	Ag_2CO_3	275.77	6.077	d 220		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	chlorate	AgClO ₃	191.34	4.430^{20}	231	d 270	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	chloride	AgCl	143.34		455	1564	0.00019 aq; s NH ₄ OH
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	chromate(VI)	Ag_2CrO_4	331.77	5.625^{25}			0.002^{20} aq; s HNO ₃ , NH ₄ OH
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	cyanide	AgCN	133.90	3.95	d 320		i aq; s KCN
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	fluoride	AgF	126.88	5.852^{16}	435	1150	172 ²⁰ aq
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	(II) fluoride	AgF_2	145.87		690	d 700	, 1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	iodate	AgIO ₃	282.80		>200		0.004^{20} aq
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	iodide	AgI					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$						d 440	1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		2					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	oxide						0.002^{25} aq
phosphate, ortho- Ag_3PO_4 418.62 6.370 849 0.006 aq	(II) oxide						
	1 0						
oulfoto A = CO 211 92 5 4530 660 41005 0.9020 ag					1		1
surface $ Ag_2SO_4 $ 511.65 5.45 600 d 1085 0.80° aq	sulfate	Ag_2SO_4	311.83	5.45^{30}	660	d 1085	$0.80^{20}\mathrm{aq}$

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sodium	Na	22.99	0.968^{20}	97.82	881.4	d aq to NaOH
acetate	NaC ₂ H ₃ O ₂	82.04	1.528	324		46.5^{20} aq
aluminate, tetrachloro-	NaAlCl ₄	191.80		151		s aq
amide	NaNH ₂	39.02		210	subl 400	d viol aq
aurate(III) dihydrate,	NaAuCl ₄ ·2H ₂ O	397.80	1.6	d 100		166 ²⁰ aq
tetrachloro-						•
azide	NaN ₃	65.01	1.846^{20}	d		41 ²⁰ aq; 0.3 alc
benzoate	NaC ₆ H ₅ O ₂	144.11				63 ²⁵ aq; 1.3 alc
bismuthate $(V)(1-)$	NaBiO ₃	280.00		d		i aq; d a
boranate	NaBH ₄	37.84	1.074	497 d		55 ²⁵ aq; 4 alc; 1.4 pyr; 5 DMF
borate, tetra-	$Na_2B_4O_7$	201.27	2.367	742.5		2.6 ²⁰ aq
borate, tetrafluoro-	NaBF ₄	109.82	2.47^{20}	384	d	108 ²⁷ aq
bromate	NaBrO ₃	150.91	3.339^{17}	380 d		36 ²⁰ aq
bromide	NaBr	102.91	3.205^{18}	747	1447	90 ²⁰ aq; 6 alc; 16 MeOH
carbonate	Na ₂ CO ₃	106.00	2.533	850.0	d	21.5 ²⁰ ; s glyc
carbonate 10-water	Na ₂ CO ₃ ·10H ₂ O	286.14	1.46	34		50 aq; s glyc
chlorate	NaClO ₃	106.45	2.489	248	d 350	96 ²⁰ aq; 0.77 alc; 25 glyc
chloride	NaCl	58.45	2.164^{20}	801	1465	36 ²⁰ aq; 10 glyc
chlorite	NaClO ₂	90.45		d 180–200		34 ¹⁷ aq
chromate(VI)	Na ₂ CrO ₄	161.97	2.723	792		84 ²⁰
citrate 2-water	$Na_3C_6H_5O_7 \cdot 2H_2O$	294.10		$-2H_2O, 150$		77 ²⁵ aq
cobaltate(III), hexanitrito-	$Na_3[Co(NO_2)_6]$	403.98				v s aq
cyanate	NaOCN	65.01	1.893^{20}	550		s aq d; 0.22° alc
cyanide	NaCN	49.02		562	1530	58.7 ²⁰ aq
cyanoborohydride	NaBH ₃ CN	62.84		d 242		(flammable solid)
dichromate(VI) 2-water	$Na_2Cr_2O_7 \cdot 2H_2O$	298.00	2.348_4^{25}	356 anhyd	d 400	208 ²⁰ aq
diethyldithiocarbamate	$NaS_2CN(C_2H_5)_2$	225.31		94 anhyd		s aq, alc

dimethylarsonate 3-water	$NaO_2As(CH_3)_2 \cdot 3H_2O$	214.03		60	$-3H_2O, 120$	200 aq; 40 alc
diphosphate(V)	$Na_4P_2O_7$	265.90	2.45	988	-	2.26 ⁰ aq
dithionate 2-water	$Na_2S_2O_6 \cdot 2H_2O$	242.13	2.189	$-2H_2O, 110$	d 267	6.05^{20} aq
dithionate(III) (hydro-	$Na_2S_2O_4$	174.13		d		22 ²⁰ aq
sulfite)	2 2 .					•
dodecylsulfate (laurate)	NaO ₃ SOC ₁₂ H ₂₅	288.38				10 aq
ethoxide	NaOC ₂ H ₅	68.06		>300		d aq; s abs alc
ethylenebis (aminodi-	$Na_4C_2H_4N_2(C_2H_3O_2)_4$	380.20				103 aq
acetate) (EDTA)						-
ethylsulfate	NaO ₃ SOC ₂ H ₅	148.11				
ferrate(II) 10-water,	$Na_4[Fe(CN)_6] \cdot 10H_2O$	484.07	1.458	$-10H_2O, 82$	d 435	18.8 ²⁰ aq
hexacyano-						
ferrate(III) 2-water,	Na ₂ [Fe(CN) ₅ NO]·2H ₂ O	297.65	1.72			40 ¹⁶ aq
pentacyanonitrosyl-						
(nitroprusside)						
fluoride	NaF	41.99	2.78	996	1787	4 ²⁰ aq; i alc
formate	NaOOCH	68.02	1.919	253 d		81 ²⁰ aq; s glyc; sl s alc
gluconate	$NaC_6H_{11}O_7$	218.13				59 ²⁵ aq; sl s alc; i eth
glycerophosphate	$Na_2C_3H_5(OH)_2PO_4$	216.03		d 130		60 aq; i alc
hydride	NaH	24.00	1.396	d 425		d viol aq, alc
hydrogen carbonate	NaHCO ₃	84.01	2.20	$-CO_2, 270$		9.6 ²⁰ aq; i alc
hydrogen phosphate	$NaH_2PO_4 \cdot H_2O$	137.99	2.040	$-H_2O, 100$	d 200	71 ^o aq
hydrate, di-						
hydrogen phosphate	$Na_2HPO_4 \cdot H_2O$	268.07	1.679	d		185 ⁴⁰ aq
7-water						
hydrogen sulfate	NaHSO ₄	120.07	2.435	315	d	28.5 ²⁵ aq; d alc
hydrogen sulfite	NaHSO ₃	104.06	1.48	d		29 aq; 1.4 alc
hydrogen sulfide 2-water	NaHS·2H ₂ O	92.09		55	d	s aq, alc, eth
hydroxide	NaOH	40.01	2.130^{25}	322	1557	108 ²⁰ aq; 14 abs alc; 24 MeOH;
						s glyc
hydroxymethanesulfinate	NaO ₂ SCH ₂ OH·2H ₂ O	154.12		63–64		v s aq; i abs alc, bz, eth
dihydrate						
hypochlorite	NaClO	74.44				53 ²⁰ aq (anhyd v expl)

 TABLE 2.1
 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sodium						
iodate	NaIO ₃	197.90	4.277 ²⁰	d		8.1 ²⁰ aq
iodite	NaI	149.92	3.667°	660	1304	178 ²⁰
lactate	NaOOCCHOHCH ₃	112.07		d		misc aq, alc
methoxide	NaOCH ₃	54.03		>300		d aq; s alc
molybdate dihydrate	Na ₂ MoO ₄ ·2H ₂ O	241.95	3.28	687	$-2H_2O, 100$	65 ²⁰ aq
nitrate	NaNO ₃	85.01	2.257	308	d 380	88 ²⁰ aq
nitrite	NaNO ₂	69.00	2.168°	271	d 320	81 ²⁰ aq
oxalate	Na ₂ C ₂ O ₄	134.01	2.27			3.4 ²⁰ aq
oxide	Na ₂ O	61.98	2.27	1132	d 1950	d aq to NaOH
perchlorate	NaClO ₄	122.44	2.499	468		201^{20}
periodate	NaIO ₄	213.91	3.86546	d 300		10.3 ²⁰ aq
peroxide	Na_2O_2	77.99	2.805	675	d	v s aq (d)
peroxoborate 4-water	NaBO ₃ ·4H ₂ O	153.88		d 60		2.5 aq
peroxodisulfate(VI)	$Na_2S_2O_8$	238.13		d		55 aq
phosphate 12-water	Na ₃ PO ₄ ·12H ₂ O	380.12	1.62	73.4	$-11H_2O, 100$	28.3 ¹⁵ aq
platinate(IV) 6-water, hexachloro-	Na ₂ PtCl ₆ ·6H ₂ O	561.88	2.50	$-6H_2O, 110$		v s aq; s alc
propionate	NaOOCCH ₂ CH ₃	96.07				100^{25} aq; 4.1^{25} alc
salicylate	NaC ₇ H ₅ O ₃	160.11				95 ²⁰ aq; 11 alc; 25 glyc
selenate(VI)	Na ₂ SeO ₄	188.94	3.098			27 ²⁰ aq
silicate, hexafluoro-	Na ₂ SiF ₆	188.05	2.679	red heat		0.44 ⁰ aq; i alc
stannate(IV) 3-water	$Na_2SnO_3 \cdot 3H_2O$	266.71		d 140		50° aq
stearate	NaOOCC ₁₇ H ₃₅	306.47		d		sl s aq
sulfate	Na ₂ SO ₄	142.06	2.664	884		19.5^{20}
sulfate 10-water	Na ₂ SO ₄ ·10H ₂ O	322.19	1.464	32.4	$-10H_2O$, 100	36 ¹⁵ aq

sulfide	Na ₂ S	78.05	1.85614	950		15.7 ²⁰ aq
sulfite	Na ₂ SO ₃	126.06	2.63315	d		26 ²⁰ aq
tartrate dihydrate	Na ₂ C ₄ H ₄ O ₆ ·2H ₂ O	230.08	1.818	$-2H_2O, 120$		29 ⁶ aq
tetraphenylborate	$NaB(C_6H_5)_4$	342.24				s aq, acet
thiocyanate	NaSCN	81.07		287		134^{20} aq
thiosulfate	Na ₂ S ₂ O ₃	158.11	2.345			s aq; i alc
thiosulfate 5-water	Na ₂ S ₂ O ₃ ·5H ₂ O	248.18	1.685	-5H2O, 100		70^{20} aq (d slowly)
tungstate(VI) dihydrate	Na ₂ WO ₄ ·2H ₂ O	329.86	3.245	$-2H_2O, 100$		880
Strontium						
carbonate	SrCO ₃	147.64	3.70	$-CO_2$, 1172		0.001 ²⁵ aq; s a
chloride	SrCl ₂	158.52	3.052	874	2058	52.9 ²⁰ aq
chromate(VI)	SrCrO ₄	203.64	3.89515			0.09 ²⁰ aq; s HCl
hydroxide	Sr(OH) ₂	121.64	3.625	375 (in H ₂)	$-H_2O,710$	1.77 ²⁰ aq
Sulfamic acid	H ₂ NSO ₃ H	97.09	2.126	d 200	2 .	14.7 ag
Sulfinyl						•
bromide	SOBr ₂	207.88	2.67	-49.5	139.7	d aq
chloride	SOCl ₂	118.98	1.65615	-104.5	75.8	hyd aq
fluoride	SOF ₂	86.06	3.0^{-44}	-110	-43.8	d aq; s bz, chl, eth
Sulfonyl	2					•
chloride	SO ₂ Cl ₂	134.98	1.667420	-46	69.3	d aq; s bz
fluoride	SO ₂ F ₂	102.07	$3.72\mathrm{g}\cdot\mathrm{L}^{-1}$	-135.8	-55.38	4 mL aq; 24 mL alc; 136 mL
						CCl ₄ ; 210 mL toluene
Sulfur	S	32.07	1.92	106.8	444.60	i aq; 23° CS ₂ ; s alc, bz
	S_8	256.51	1.96^{20}	115.21	444.60	i aq; 23° CS ₂ ; s alc, bz
(di-) chloride, di-	S ₂ Cl ₂	135.03	1.688_{15}^{15}	-80	138.1	hyd aq
fluoride, tetra-	SF ₄	108.07	1.919^{-73}	-121	-38	d viol aq; s bz
fluoride, hexa-	SF ₆	146.07	1.88^{-50}	-50.8	subl 63.8	sl s aq; s alc, KOH
			$g \cdot L^{-1}$			-
oxide, di	SO ₂	64.07	2.716^{20}	-75.47	-10.01	3937 ²⁰ mL aq; 25 mL alc
	_		$g \cdot L^{-1}$			_
			1.46 ⁻¹⁰ (lq)			
oxide, tri(III)	SO_3	80.07	1.9225^{20}	16.86	43.4	slowly v s aq

TABLE 2.1 Physical Constants of Inorganic Compounds (continued)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sulfuric acid	H ₂ SO ₄	98.08	1.831820	10.38	335.5	v s aq
chloro-	HOSO ₂ C1	116.52	1.753^{20}	-80	152	d viol aq
fluoro-	FSO ₂ OH	100.07	1.726^{25}	-88.98	162.6	d viol aq
Tantalum	Ta	180.95	16.69	2985	5513	i aq; s HF, fused alk
(V) fluoride	TaF ₅	275.95	4.74 ²⁰	95–97	229	s aq
Tellurium	Te	127.60	6.24 ²⁰	450	1009	i aq; s HNO3, KOH
Thallium	Tl	204.37	11.85	303.5	1487	i aq; s HNO ₃
(III) acetate sesquihydrate	$TI(C_2H_3O_2)_3 \cdot 1.5H_2O$	408.53		182 d		
(I) bromide	TlBr	284.31	7.54	460	825	0.05 ²⁰ aq; s alc
(I)chloride	TICI	239.85	7.004^{30}	429	816	0.33 ²⁰ aq
(I) ethoxide	TlOC ₂ H ₅	249.43	3.493^{20}	-3	d 130	sl s alc; s eth
(I) fluoride	TIF	223.39	8.23 ⁴	322	700	78 ¹⁵ aq
(I) nitrate	TINO ₃	266.40	5.556	206	430	9.6 ²⁰ aq
(III) nitrate 3-water	$Tl(NO_3)_3 \cdot 3H_2O$	444.43		102-103		s aq
(I) oxide	Tl ₂ O	424.78	9.5216	300	1080	v s aq (d); s a
(III) oxide	Tl_2O_3	456.78	10.19 ²² (hex)	717	$-O_2, 875$	i aq; s a
(I) sulfate	Tl ₂ SO ₄	504.85	6.77	632	d	4.9 ²⁰ aq
Thiocarbonyl chloride	CSCl ₂	114.98	1.50915		73.5	d ag; s eth
Thiocyanogen	(SCN) ₂	116.16		ca -2		d aq; s alc, CS ₂ , eth
Thionyl, see Sulfinyl	, ,,2					1
Tin (silver-white, tetr)	Sn	118.69	7.28	231.89	2623	i aq; s HCl, H ₂ SO ₄
(gray, cub)			5.75	stable -161 to 13.2		
(IV) bromide	SnBr₄	438.36	3.35^{33}	30	207	hyd aq; s acet
(II) chloride	SnCl ₂	189.61	3.95	247	652	84° aq; s alc, eth

(IV) chloride (II) diphosphate(V) (II) fluoride (IV) fluoride (IV) oxide (II) sulfide (IV) sulfide (IV) sulfide (IV) sulfide	SnCl ₄ Sn ₂ P ₂ O ₇ SnF ₂ SnF ₄ SnO ₂ SnS SnS ₂ SnZrF ₆	260.53 411.32 156.70 194.70 150.70 150.77 182.83 323.92	2.226 4.009 ¹⁶ 4.57 ²⁵ 4.780 ¹⁹ 6.95 5.08 4.5 4.21	-34 213 subl 705 1630 881 765	subl 1900 1210	s aq, eth i aq; s conc a 30 aq hyd aq i aq i aq; s conc HCl i aq; d by aqua regia
hexafluoro-	SHZIT'6	323.92	4.21			s aq
Titanium (III) chloride	Ti TiCl ₃	47.90 154.27	4.507 2.71	1660 subl 831 (vac)	3318 d 5000	s hot a, HF s aq, alc
(IV) chloride hydride, di	TiCl ₄ TiH ₂	189.73 49.92	1.726 3.752	-24.10 d 400	136.4	s cold aq, alc
(IV) isopropoxide (IV) oxide (rutile) (III) sulfate	Ti[OCH(CH ₃) ₂] ₄ TiO ₂ Ti ₂ (SO ₄) ₃	284.26 79.90 384.00	0.9711^{20} 4.23	ca 20 1857	220 ^{10 mm}	s HF s HCl
Trisulfuryl dichloride	CISO,OSO,OSO,CI	295.09	1.90^{20}	18.7	61 ^{3 mm}	
Tungsten						
(VI) chloride	WCl ₆	396.57	2.721^{282}	281.5	340.5	hyd aq; s CS ₂ , CCl ₄
(VI) oxide	WO_3	231.86	7.16	1472	1837	i aq; s hot alk
sulfide, di-	WS_2	247.98	7.5^{10}	d 1250		$s HNO_3 + HF$
Uranyl			- 00-15			15
(VI) acetate 2-water	$UO_2(C_2H_3O_2)_2 \cdot 2H_2O$	422.13	2.89315	$-2H_2O, 110$	d 275	7.7 ¹⁵ aq
nitrate 6-water	$UO_2(NO_3)_2 \cdot 6H_2O$	502.13	2.807^{13}	60.2	d 100	155 ²⁰ aq
Vanadium	N.O.	1.40.00	4.87	2067		' IDIO - HE
(III) oxide	V_2O_3	149.00 181.90	3.35	670	1690	i aq; s HNO ₃ + HF
(V) oxide (IV) oxide sulfate	V ₂ O ₅	163.00	3.33	670	1090	0.80 aq; s a, alk
Xenon	VOSO ₄ Xe	131.30	5.8971°	-111.8	-108.10	v s aq 10.8 ²⁰ mL aq
ACHUII	Ac	131.30	g•L ⁻¹	-111.0	-106.10	10.6 IIIL aq
fluoride, di-	XeF ₂	169.30	3.13^{25}	129.0	subl 114	2.5° aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Xenon						
fluoride, tetra-	XeF ₄	207.30	3.03^{25}	117.1	subl 116	hyd aq; s F ₃ CCOOH
fluoride, hexa-	XeF ₆	245.30	3.411^{25}	49.5	75.6	hyd aq
Zinc	Zn	65.37	7.14^{25}	419.6	911	i aq; s a, alk
acetate dihydrate	$Zn(C_2H_3O_2)_2 \cdot 2H_2O$	219.49	1.735	237		41.6 ²⁰ aq; 3.3 alc
bromide	ZnBr ₂	225.21	4.22	402	650	446 ²⁰ aq; 200 alc; s eth
carbonate	ZnCO ₃	125.38	4.398	$-CO_2, 300$		0.02 ²⁵ aq; s a, alk
chloride	ZnCl ₂	136.29	2.907^{25}	318	732	395 ²⁰ aq; 77 alc; 50 glyc
chromate(VI)	ZnCrO ₄	181.36	3.40			i aq; s a
cyanide	Zn(CN) ₂	117.42	1.852	d 800		0.05818 aq; s KCN, alk
fluoride	ZnF_2	103.38	5.00^{25}	872	1500	1.6 ²⁰ aq
iodide	ZnI_2	319.22	4.736^{25}	446	730	432 ²⁰ aq; 50 glyc
nitrate 6-water	$Zn(NO_3)_2 \cdot 6H_2O$	297.47	2.065^{14}	36.4	$-6H_2O$, 131	146º aq
oxide	ZnO	81.37	5.67	1970		i aq; s a, alk
peroxide	ZnO_2	97.38	3.00	d 150		i aq; d slowly
p-phenolsulfonate 8-water	$Zn[C_6H_4(OH)SO_3]_2 \cdot 8H_2O$	555.83		$-8H_2O, 120$		63 aq; 56 alc
phosphate(V)	$Zn_2(PO_4)_2$	386.05	3.998^{15}	900		i aq; s a, NH ₄ OH
phosphide	Zn_3P_2	258.09	4.55	>420	subl 1100 (in H_2)	d aq; s bz, CS ₂ ; d viol HCl
propionate	Zn(OOCCH ₂ CH ₃) ₂	211.52				32 aq; 2.8 alc
silicate 6-water, hexafluoro-	ZnSiF ₆ ·6H ₂ O	315.54	2.104	d 100		v s aq
stearate	$Zn(OOCC_{17}H_{35})_2$	632.33		ca 120		i aq, alc, eth; s bz
sulfate	ZnSO ₄	161.44	3.54	1200		53.8 ²⁰ aq
sulfate 7-water	ZnSO ₄ ·7H ₂ O	287.54	1.957	$-7H_2O, 280$	d 500	96 ²⁰ aq; 40 glyc; i alc
sulfide	ZnS	97.43	4.087	1722		i aq; s a
thiocyanate	Zn(SCN) ₂	181.53				0.14 ¹⁸ aq; s alc

Zirconium	Zr	91.22	6.52^{30}	1852	4504	s aqua regia
(IV) chloride	ZrCl ₄	233.05	2.803^{15}	437	subl 334	hyd aq; s alc, eth
chloride oxide 8-water	ZrCl ₂ O·8H ₂ O	322.25	1.91	$-8H_{2}O, 210$		s aq
hydroxide	Zr(OH) ₄	159.25	3.25	$-2H_2O, 500$		s a
(IV) oxide	ZrO ₂	123.22	5.85	2677	4275	s hot H ₂ SO ₄ , HF slowly
silicate(4-)	ZrSiO ₄	183.31	4.56	d 1538		very inert
sulfate 4-water	$Zr(SO_4)_2 \cdot 4H_2O$	355.41	3.22^{16}	anhyd 380		52.5 ¹⁸ aq

SECTION 3

PROPERTIES OF ATOMS, RADICALS, AND BONDS

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3.2 SECTION 3

NUCLIDES

TABLE 3.1 Table of Nuclides

Explanation of column headings

Nuclide. Each nuclide is identified by its atomic number Z, equal to the number of protons in the nucleus; the corresponding symbol for that element; and the mass number A, equal to the sum of the numbers of protons Z and neutrons N in the nucleus. Thus, A = Z + N, or N = A - Z. The m following the mass number (e.g., ^{69}m Zn) indicates an isomer of that nuclide.

Half-Life. For the radioactive nuclides this time period corresponds to that during which loss by disintegration of 50% of the nuclide occurs. The units of time are designated by year (yr), day (d), hour (h), minute (min), and second (s).

Natural Abundance. The isotopic abundances listed are on an "atom percent" basis for the stable nuclides present in naturally occurring elements in the earth's crust.

Thermal Neutron Absorption Cross Section. The ease with which a given nuclide can absorb a thermal neutron (energy $\leq \frac{1}{40}$ eV) and become of a different nuclide is indicated by the cross section, given here in units of barns (1 barn = 10^{-24} cm²). If the mode of reaction is other than (n, γ) , it is so indicated, for example, (n, p) or (n, α) , where n = neutron, p = proton, $\gamma = \text{gamma ray}$, and $\alpha = \text{alpha particle (}^4_{\text{He}})$.

Major Radiations. In this column are listed the principal mode(s) of decay and the energies of the emanating radiations in million electronvolts (MeV). The gamma-ray (γ) intensities, where given, are given to the nearest whole percentage in parentheses following the numerical energy value for that particular γ . In most cases the radiations listed should be sufficient for identification of the particular nuclide. The following designations are used: negatron (β ⁻), positron (β ⁺), conversion electron (e⁻), gamma ray (γ), and alpha particle (α).

Ni	ıclide		Natural	Thermal neutron absorption	
Symbol	Mass	Half-life	abundance, %	cross section, barns	Major radiations
¹ H	1.007 825		99.985	0.332	
^{2}H	2.014 102		0.015	0.0005	
^{3}H	3.016 050	12.26 yr			β^{-} , 0.018 6; no γ
⁶ Li	6.015 125		7.42	$953(n,\alpha)$	
⁷ Li	7.016 004		92.58	0.037	
⁷ Be	7.016 929	53.6d		54,000(n, p)	γ , 0.477(10)
Ве	9.012 186		100	0.009	
¹⁰ Be	10.013 534	$2.5 \times 10^{6} \text{yr}$			β^{-} , 0.555; no γ
^{10}B	10.012 939		19.7	$3837(n,\alpha)$	
^{11}B	11.009 305		80.3	0.005	
¹¹ C	11.011 432	20.34 min			β^+ , 0.97; γ , 0.511
¹³ C	13.003 354		1.108	0.0009	
¹⁴ C	14.003 242	5730 yr			β^{-} , 0.156; no γ
¹³ N	13.005 738	9.96 min			β^+ , 1.20; γ , 0.511
¹⁴ N	14.003 074		99.635	1.81(n, p)	
¹⁹ O	19.003 578	29.1 s			β^- , 4.60; γ , 0.197(97), 1.37(59)
¹⁸ F	18.000 937	109.7 min			β^+ , 1.74; γ , 0.511
²² Na	21.994 437	2.62 yr			β^+ , 1.820, 0.545; γ , 0.511, 1.275(100)

TABLE 3.1 Table of Nuclides (*continued*)

Nuclide			Natural abundance,	neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
²³ Na	22.934 473		100	0.53	
²⁴ Na	23.990 962	14.96h			β^- , 4.17, 1.389;
²⁵ Mg	24.985 839		10.11	0.3	γ, 0.511, 1.275(100)
²⁸ Mg	27.983 875	21.2h	10.11	0.3	$\beta^-, 0.46; e^-, 0.03;$
6	27,500 070	21.21			γ, 0.031(96), 0.40(30), 0.95(30), 1.35(70)
²⁶ A1	25.986 891	$7.4 \times 10^5 \text{yr}$			β^- , 8.5; γ , 0.511, 1.12(4), 1.81(100)
²⁷ Al	26.981 539		100	0.235	
²⁸ Al	27.981 905	2.31 min			$\beta^-, 2.85; \gamma, 1.780$ (100)
³⁰ Si	29.973 763		3.12	0.11	
³¹ Si	30.975 349	2.62h	100	0.10	β^- , 1.48; γ , 1.26
³¹ P ³² P	30.973 765	14 20 4	100	0.19	0= 1.710
³³ P	31.973 909 32.971 728	14.28d 24.4d			$\beta^-, 1.710$ $\beta^-, 0.248; \text{ no } \gamma$
³⁴ S	33.967 865	24.44	4.22	0.27	ρ ,0.240,110 γ
³⁵ S	34.969 031	87.9 d	7.22	0.27	β^- , 0.167; no γ
^{38}S	37.971 230	2.87h			$\beta^-, 3.0, 1.1;$
					γ, 1.88(95)
³⁵ Cl	34.968 851	_	75.53	44	
³⁶ Cl	35.968 309	$3.08 \times 10^{5} \text{yr}$		100	β^- , 0.714; γ , 0.511
³⁷ Cl ³⁸ Cl	36.965 898 37.968 005	37.29 min	24.47	0.4	0= 4.01, 1.60(20)
³⁹ Cl	38.968 003	55.5 min			$\beta^-, 4.91; \gamma, 1.60(38)$ $\beta^-, 3.45, 2.18,$
CI	36.708 000	33.311111			1.91; γ, 0.246(44)
³⁷ Ar	32.966 772	35.1 d			Cl X rays
⁴⁰ K	39.964 000	$1.26 \times 10^9 \mathrm{yr}$	0.118	70	β^- , 1.314; β^+ , 0.483; γ , 1.460(11)
⁴¹ K	40.961 832		6.77	1.2	·
⁴² K	41.962 406	12.36h			β^- , 3.52; γ , 0.31,
110	12.055.100		200		1.524(18)
⁴⁴ Ca ⁴⁵ Ca	43.955 490 44.956 189	165 d	2.06	0.7	0- 0.252
⁴Ca ⁴7Ca	46.954 538	4.535 d			$\beta^-, 0.252$ $\beta^-, 1.98, 0.67;$
Ca	40.934 338	4.555 u			$ \rho, 1.98, 0.07, \\ \gamma, 0.49(5), \\ 0.815(5), $
					1.308(74)
⁴⁶ Sc	45.955 919	83.9 d			β^- , 1.48, 0.357, γ , 0.889(100),
					1.120(100)

3.4 SECTION 3

TABLE 3.1 Table of Nuclides (*continued*)

N	uclide		Natural abundance,	neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
⁴⁴ Ti	43.959 572	48 yr			γ, 0.068(90), 0.078(98); e ⁻ , 0.065, 0.073
^{48}V	47.952 259	16.0d			β^+ , 0.696; γ , 0.511, 0.945(10), 0.983(100), 1.312(97), 2.241(3)
⁴⁹ V ⁵⁰ Cr	48.949 522 49.946 054	330d	4.31	17	Ti X rays
51Cr	50.944 768	27.8d	4.31	17	γ , 0.320(9); e^- , 0.315
⁵⁴ Mn	53.940 362	303 d			γ , 0.320(9), ϵ , 0.313 γ , 0.835(100);
14111	33.740 302	303 u			$e^-, 0.829$
⁵⁵ Mn	54.938 050		100	13.3	c , 0.02)
⁵⁶ Mn	55.938 910	2.576h	100	10.0	$\beta^-, 2.85;$
					γ, 0.847(99), 1.811(29), 2.110(15)
⁵⁴ Fe	53.939 617		5.84	2.9	
⁵⁵ Fe	54.938 299	2.60 yr			Mn X rays
⁵⁸ Fe	57.933 282		0.31	1.1	
⁵⁹ Fe	58.934 878	45.6d			β^- , 1.57, 0.475;
					γ , 0.143(1),
					0.192(3),
					1.095(56),
					1.292(44)
⁵⁷ Co	56.936 296	270d			γ , 0.014(9), 0.122(87),
					0.136(11), 0.692;
⁵⁸ Co	57.025.761	71.2.1			e ⁻ , 0.115, 0.129
Co	57.935 761	71.3 d			β^+ , 0.474; γ , 0.511,
					0.810(99), 0.865(1), 1.67(1)
⁵⁹ Co	58.933 189		100	19	1.07(1)
⁶⁰ Co	59.933 813	5.263 yr	100	6	β^- , 1.48, 0.314;
Co	37.733 013	3.203 J1			γ , 1.173(100),
					1.332(100)
⁶² Ni	61.928 342		3.66	15	
⁶³ Ni	62.929 664	92 yr			β^{-} , 0.067; no γ
⁶⁴ Ni	63.927 958		1.16	1.5	,
⁶⁵ Ni	64.930 072	2.564h			β^- , 2.13; γ , 0.368(5),
					1.115(16), 1.481(25)
⁶³ Cu	62.929 592		69.1	4.5	
⁶⁴ Cu	63.929 759	12.80h			$\beta^-, 0.573; \beta^+, 0.656;$ $e^-, 1.33;$
					γ , 0.511, 1.34(1)

TABLE 3.1 Table of Nuclides (*continued*)

Ni	uclide		Natural abundance,	Thermal neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
⁶⁴ Zn	63.929 145	$> 8 \times 10^{15} \text{yr}$	48.89	0.46	
⁶⁵ Zn	64.929 234	245 d			$\beta^+, 0.327; e^-, 1.106;$ $\gamma, 0.511, 1.115(49)$
⁶⁸ Zn ⁶⁹ <i>m</i> Zn	67.924 857	13.8h	18.56	1.0	2. 0 420(05). 2
		13.611			γ, 0.439(95); e ⁻ , 0.429
⁷¹ Ge	70.924 956	11.4d	100	4.5	Ga X rays
⁷⁶ As	74.921 595 75.922 397	26.4h	100	4.3	$\beta^-, 2.97; \gamma, 0.559(43),$
					0.657(6), 1.22(5) 1.44(1), 1.789, 2.10(1)
⁷⁷ As	76.920 645	38.7 h			$\beta^-, 0.68; \gamma, 0.086,$
⁷⁵ Se	74.922 525	120.4 d			0.239(3), 0.522(1) γ, 0.066(1), 0.097(1), 0.121(17),
					0.121(17), 0.136(57),
					0.265(60), 0.280(25),
					$0.401(12)$; $e^-0.085$,
					0.095, 0.109, 0.124, 0.253
⁷⁹ Br ⁸⁰ Br	78.918 329 79.918 536	17.6 min	50.52	8.5	$\beta^-, 2.00; \beta^+, 0.87;$
DI	79.910 330	17.0111111			γ , 0.511, 0.618(7),
⁸¹ Br	90.016.202		49.48	3	0.666(1)
82Br	80.916 292 81.916 802	35.34h	49.46	3	$\beta^{-}, 0.444;$
					γ, 0.554(66),
					0.619(41), 0.698(27),
					0.076(27), 0.777(83),
					0.828(25),
					1.044(29), 1.317(26), 1.475(17)
⁸⁵ Kr	84.912 523	10.76 yr		<15	$\beta^-, 0.67; \gamma, 0.514$
⁸⁶ Rb	85.911 193	18.66 d			β^- , 1.78; γ , 1.078(9)
⁸⁵ Sr	84.912 989	64.0 d			γ , 0.514(100); e^- , 0.499
⁹⁰ Y	89.907 163	64.0 h		_	β^- , 2.27; no γ
⁹⁵ Nb	94.906 832	35.0d		~7	$\beta^-, 0.160;$ $\gamma, 0.765(100)$

3.6 SECTION 3

TABLE 3.1 Table of Nuclides (*continued*)

Nı	uclide		Natural abundance,	Thermal neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
⁹⁹ Mo ^{99 m} Tc ¹⁰³ Ru	98.907 720 102.906 306	66.7h 6.049h 39.5 d			β^- , 1.23; γ , 0.041(12), 0.181(7), 0.372(1), 0.740(12), 0.780(4) γ , 0.140(90); e^- , 0.110 β^- , 0.70, 0.21; γ , 0.497(88), 0.610(6)
¹⁰⁸ Pd ¹⁰⁹ Pd	107.903 891 108.905 954	13.47h	26.7	12	β ⁻ , 1.028; γ, 0.088(5), 0.129, 0.31, 0.41, 0.60, 0.64
¹⁰⁹ Ag ¹¹⁰ mAg	108.904 756	39.2s	48.65	89	γ , 0.088(5)
¹¹¹ Ag ¹⁰⁹ Cd ¹¹⁵ Cd	110.905 316 108.904 928 114.905 431	7.5 d 453 d 53.5 h			β^- , 1.05; γ , 0.247(1), 0.342(6) γ , 0.088; e^- , 0.062 β^- , 1.11; γ , 0.230(1), 0.262(2), 0.49(10),
¹¹³ <i>m</i> In		99.8 min			0.53(26) γ, 0.393(64); e ⁻ , 0.365, 0.389
¹¹⁴ In	113.904 905	72 s			β^- , 1.988; β^+ , 0.42; γ , 1.299
¹¹³ Sn ¹²¹ Sb ¹²² Sb	112.905 187 120.903 816 121.905 183	115d 2.80d	57.25	6	γ , 0.255(2) β^- , 1.97; β^+ , 0.56; γ , 0.584(66), 0.686(3), 1.14(1)
¹²³ Sb ¹²⁴ Sb	122.904 213 123.905 973	1.3×10 ¹⁶ yr 60.4 d	42.75	3.3 2000	1.26(1) β^- , 2.31; γ , 0.603(97), 0.644(7), 0.72(14), 0.967(2), 1.048(2), 1.31(3), 1.37(5), 1.45(2), 1.692(50),
¹²⁵ Sb	124.905 232	2.71 yr		<20	2.088(7) β^- , 0.61; e^- , 0.114, 0.395; γ , 0.176(6), 0.427(31), 0.463(10), 0.599(24), 0.634(11), 0.66(3)

TABLE 3.1 Table of Nuclides (*continued*)

Nuclide			Natural abundance,	Thermal neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
¹³² Te	131.908 523	77.7 h			β ⁻ , 0.22; e ⁻ , 0.197; γ, 0.053(17), 0.230(90)
^{125}I	124.904 578	60.2 d		9	γ , 0.035(7); e^- , 0.030
¹²⁷ I ¹²⁸ I	126.904 470 127.905 838	24.99 min	100	6.4	β^- , 2.12; γ , 0.441(14), 0.528(1), 0.743, 0.969
¹³¹ I	130.906 127	8.05 d		~0.7	β ⁻ , 0.806, 0.606; e ⁻ , 0.330; γ, 0.080(3), 0.284(5), 0.364(82), 0.637(7), 0.723(2)
¹³² I	131.907 981	2.26h			β^- , 2.12; γ , 0.24(1), 0.52(20), 0.67(44), 0.773(89), 0.955(22) 1.14(6), 1.28(7), 1.40(14), 1.45(1), 1.91(1), 1.99(1)
¹³³ Xe	132.905 815	5.270 d		190	$\beta^-, 0.346; e^-, 0.045, 0.075; \gamma, 0.081(37)$
¹³¹ Cs ¹³⁴ Cs	130.905 466 133.906 823	9.70 d 2.046 yr		136	Xe X rays β^- , 0.662; γ , 0.57(23), 0.605(98), 0.796(99), 1.038(1), 1.168(2),
¹³⁷ Cs	136.906 770	30.0 yr		0.11	1.365(3) β^- , 1.176, 0.514; e^- , 0.624, 0.656; γ , 0.662(85)
¹³¹ Ba	130.906 716	12.0 d			γ, 0.002(83) γ, 0.124(28), 0.216(19), 0.25(5), 0.373(13), 0.496(48), 0.60(3); e ⁻ , 0.118, 0.180, 0.460
¹³³ Ba	132.905 879	7.2 yr			γ, 0.080(36), 0.276(7), 0.302(14), 0.356(69), 0.382(8); e ⁻ , 0.266, 0.319

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 TABLE 3.1
 Table of Nuclides (continued)

Nuclide		Natural abundance		Thermal neutron absorption cross section,	
Symbol	Mass	Half-life	%	barns	Major radiations
^{137m} Ba		2.554 min			γ , 0.662(89); e^- ,
¹⁴⁰ Ba	139.910 565	12.80 d		<20	0.624, 0.656 β^- , 1.02; γ , 0.030(11), 0.163(6), 0.305(6),
¹⁴¹ Ce	140.908 219	32.5 d		30	0.438(5), 0.537(34) β^- , 0.581; e^- , 0.104, 0.139;
¹⁴⁴ Ce	143.913 591	284 d		1.0	$ \gamma, 0.145(48) $ $ \beta^-, 0.31; \gamma, 0.080(2), $ $ 0.134(11) $
¹⁹⁷ Au	196.966 541		100	98.8	
¹⁹⁸ Au	197.968 231	2.697 d		26,000	β^- , 0.962; e^- , 0.329, 0.398; γ , 0.412(95), 0.676(1), 1.088
¹⁹⁹ Au	198.968 773	3.15 d		~30	β^- , 0.46, 0.30; γ , 0.158(37), 0.208(8); e^- , 0.125, 0.145
¹⁹⁷ Hg	196.967 360	65 h			γ, 0.77(18), 0.191(2), 0.268
²⁰³ Hg	202.972 880	46.9 d			β ⁻ , 0.214; e ⁻ , 0.194, 0.264, 0.275; γ, 0.279(77)
²⁰³ Tl	202.972 353		29.50	11	,,
²⁰⁵ Tl	203.973 865	3.81 yr			$\beta^-, 0.766$
²¹⁰ Pb	209.984 187	20.4 yr			$\beta^-, 0.061; \gamma, 0.047(4);$
					$\alpha, 3.72$
²⁰⁷ Bi	206.978 438	30.2 yr			γ, 0.570(98), 1.063(77),
					1.771(9); e ⁻ 0.482, 0.975,
²¹⁰ Po	209.982 876	138.40d		< 0.03	1.048 α , 5.305; γ , 0.803
²²⁶ Ra	226.025 360	1602 yr		20	α , 4.78, 4.60;
					γ , 0.186(4), 0.26, 0.42, 0.61; e^- , 0.170
²⁴¹ Am	241.056714	433 yr		700	α, 5.49, 5.44; γ, 0.060(36), 0.101, 0.208, 0.335, 0.37, 0.663, 0.722

ELECTRONEGATIVITY

According to Pauling, electronegativity χ is the relative attraction of an atom for the valence electrons in a covalent bond. It is proportional to the effective nuclear charge and inversely proportional to the covalent radius.

$$\chi = \frac{0.31(n+1\pm c)}{r} + 0.50$$

where n is the number of valence electrons, c is any formal valence charge on the atom and the sign before it corresponds to the sign of this charge, and r is the covalent radius. Because electronegativity is concerned with atoms in molecules rather than atoms in isolation, it is not possible to define precise electronegativity values. Pauling determined his set of values from bond energy data based on experimentally measured heats of dissociation and formation. Originally the element fluorine, whose atoms have the greatest attraction for electrons, was given an arbitrary electronegativity of 4.0. A revision of Pauling's values based on newer heat data assigns 3.9 to fluorine. A unit positive charge changes the χ value for an atom by about two-thirds of the electronegativity difference between it and the atom next on its right in the Periodic Table, and a unit negative charge similarly decreases the χ value.

The greater the difference in electronegativity, the greater is the ionic character of the bond. The amount of ionic character I is given by the expression

$$I = 1 - e^{-0.25(\chi_{A} - \chi_{B})2}$$

The bond is fully covalent when $(\chi_A - \chi_B) < 0.5$ (and I < 6%). A different expression was proposed by Hannay-Smyth.*

$$I = 0.46|\chi_{A} - \chi_{B}| + 0.035(\chi_{A} - \chi_{B})^{2}$$

Other sets of electronegativities of the elements have been proposed. The rather direct, but somewhat limited, method of Mulliken makes use of the ionization potential IP and electron-affinity data (Table 3.3). Numerical values are obtained that coincide with values from other methods if electronegativities are calculated from

$$\chi = \frac{IP + A}{5.6}$$

Electronegativities on the Allred-Rochow scale[†] are given by

$$\chi = 0.359 \frac{Z_{\text{eff}}}{r^2} + 0.744$$

where Z_{eff} is the effective nuclear charge and r is the atomic radius.

Using Pauling's values, electronegativities of the elements are arranged in periodic order in Table 3.2A.

^{*} Hannay-Smyth, J. Am. Chem. Soc., 68: 171 (1946).

[†] J. Inorg. Nucl, Chem., 5: 264, 269 (1958).

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TABLE 3.2A Electronegativities of the Elements

H 2.2												
Li 1.0	Be 1.5							B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2							Al 1.5	Si 1.8	P 2.1	S 2.4	Cl 2.8
K 0.9	Ca 1.0	Sc 1.3	Ti–V 1.6	Cr–Mn 1.6	Fe–Ni 1.8	Cu 1.9	Zn 1.7	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.7
Rb 0.8	Sr 1.0	Y 1.2	Zr–Nb 1.6	Mo-Tc 1.8	Ru–Pd 2.2	Ag 1.9	Cd 1.5	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.2
Cs	Ba	La–Lu	Hf–Ta	W-Re	Os-Pt	Au	Hg	T1	Pb	Bi		
0.7	0.9	1.1	1.3	1.8	2.2	2.4	1.4	1.8	1.8	1.9		

TABLE 3.2B Electronegativities of the Groups

Group	χ	Group	χ	Group	χ
F	4.0	ОН	3.7	C≡N	3.3
Cl	2.8	OCH ₃	3.7	C≡CH	3.3
Br	2.7	NO_2	3.4	$CH = CH_2$	3.0
I	2.2	NH ₂	3.4	C_6H_5	3.0
CF ₃	3.4	$N(CH_3)_2$	3.0	COOH	2.8
CCl ₃	3.0			SiH ₃	2.2
CHCl ₂	2.8			PH ₂	2.3
2				SH	2.8

Electronegativities have important uses in chemistry in addition to predicting the amount of ionic character in a bond. The bond stretching force constant k (in units of 10^5 dynes \cdot cm⁻¹) can be estimated for stable molecules exhibiting their normal covalences by the expression:

$$k = 1.67 N \left(\frac{\chi_{\rm A} \chi_{\rm B}}{d^2} \right)^{3/4} + 0.30$$

where N is the bond order (i.e., the effective number of covalent or ionic bonds acting between the two atoms A and B) and d is the internuclear distance in angstroms.

An estimate of the percent ionic character may be made for organometallic compounds of the type alkyl-metal for metals in common use in organic synthesis. Among the alkali metals (row 1 of the Periodic Table, these are Li (43%), Na (47%), and K (51%)). The percent ionic character for an organomagnesium compound (typically a Grignard reagent), the bond is estimated to be 34% ionic. The more covalent organozinc and organocadmium compounds have correspondingly less ionic character: Zn (18%) and Cd (15%).

Electronegativities have also been estimated for various common substituent groups. They are arranged in Table 3.2B in clusters of related residues. The values for the individual halogens are from Table 3.2A.

Electronegativity is proportional to the work function ϕ , which is the energy necessary to just remove an electron from the metal surface in thermoelectric or photoelectric emission.

$$\chi = 0.44 \phi - 0.15$$

ELECTRON AFFINITY

The *electron affinity* of an atom A is defined as the energy released when an atom and an electron react to form a negative ion in the gas phase at 0 K.

$$A(g) + e^- = A^-(g)$$

An example is the capture of an electron by chlorine to give chloride anion.

$$Cl(g) + e^- = Cl^-(g)$$
.

Conceptually related to this is the *ionization potential*, which is the energy for the process

$$A \rightarrow A^+ + e^-$$
.

An example is the loss of an electron by an alkali metal to give the alkali metal cation.

$$Na \rightarrow Na^+ + e^-$$

The second ionization potential carried this process further, that is, $A^+ \to A^{2+} + e^-$ and so on for the third or more ionization potentials. Both electron affinities and ionization potentials are typically expressed in electron volts (eV). Data for electron affinities are given in Table 3.3. Uncertainty in the final data figures is given in parentheses.

Source: H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 4: 539 (1975). Data for ionization potentials are available in C. E. Moore, National Bureau of Standards U. S. Publication NSRDS-NBS, 34 (1970).

 TABLE 3.3
 Electron Affinities of Elements, Molecules and Radicals

A. Elements

Element	Electron affinity, eV*	Element	Electron affinity, eV*
Aluminum Antimony Argon Arsenic Astatine Barium	0.46(3)	Beryllium	<0
	1.05(5)	Bismuth	1.1(2)
	< 0	Boron	0.28(1)
	0.80(5)	Bromine	3.364(4)
	2.8(2)	Cadmium	<0
	< 0	Calcium	<0

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 TABLE 3.3
 Electron Affinities of Elements, Molecules and Radicals (continued)

A. Elements

		I	
Element	Electron affinity, eV*	Element	Electron affinity, eV*
Carbon	1.268(5)	Oxygen	1.462(3)
Cesium	0.4715(5)	Palladium	0.6(3)
Chlorine	3.615(4)	Phosphorus	0.743(10)
Chromium	0.66(5)	Platinum	2.128
Cobalt	0.7(2)	Polonium	1.9(3)
Copper	1.226(10)	Potassium	0.5012(5)
Fluorine	3.399(3)	Radon	<0
Francium	(0.456)	Rare earths	≤0.5 (estimate)
Gallium	0.30(15)	Rhenium	0.15(10)
Germanium	1.2(1)	Rhodium	1.2(3)
Gold	2.3086(7)	Rubidium	0.4860(5)
Hafnium	>0	Ruthenium	1.1(3)
Helium	<0	Scandium	<0
Hydrogen	0.754 209(3)	Selenium	2.0206(3)
Indium	0.30(15)	Silicon	1.385(5)
Iodine	3.061(4)	Silver	1.303(7)
Iridium	1.6(2)	Sodium	0.546(5)
Iron	0.25(20)	Strontium	<0
Krypton	<0	Sulfur	2.0772(5)
Lanthanum	0.5(3)	Tantalum	0.6(4)
Lead	1.1(2)	Technetium	0.7(3)
Lithium	0.620(7)	Tellurium	1.9708(3)
Magnesium	<0	Thallium	0.3(2)
Manganese	<0	Tin	1.25(10)
Mercury	<0	Titanium	0.2(2)
Molybdenum	1.0(2)	Tungsten	0.6(4)
Neon	<0	Vanadium	0.5(2)
Nickel	1.15(10)	Xenon	<0
Niobium	1.0(3)	Yttrium	0.0(3)
Nitrogen	-0.07(8)	Zinc	≈0
Osmium	1.1(3)	Zirconium	0.5(3)

B. Molecules

Molecule	Electron affinity, eV*	Molecule	Electron affinity, eV*
BF_3	2.65	SF ₆	1.43
<i>p</i> -Benzoquinone	1.34	2,3,5,6-Tetrachloro-	2.40
NO_2	3.91	benzoquinone	
O_2	0.45	Tetracyanoethylene	2.88

^{*} To convert into kJ \cdot mol⁻¹ multiply by 96.48. To convert into kcal \cdot mol⁻¹ multiply by 23.06.

TABLE 3.3 Electron Affinities of Elements, Radicals and Molecules (*continued*)

C. Radicals

Radical	Electron affinity, eV*	Radical	Electron affinity, eV*
CH ₃	1.08	ОН	1.83
C_2H_5	0.89	CF ₃ O	1.35
C_6H_5	2.20	CH ₃ O	0.38
CCl ₃	1.22	PH_2	1.60
CF ₃	1.85	SH	2.19
CN	3.17	CH ₃ S	1.32
NH_2	1.12	SCN	2.17
C ₆ H ₅ NH	1.55	SeCN	2.64
$(C_6H_5)_2N$	1.19	SiF_3	3.35

^{*} To convert into kJ \cdot mol⁻¹ multiply by 96.48. To convert into kcal \cdot mol⁻¹ multiply by 23.06.

BOND LENGTHS AND STRENGTHS

The bonds most commonly encountered in organic chemistry are those between carbons and between carbon and heteroatoms of the first row of the Periodic Table. Generally and very approximately, single bonds between two carbon atoms are about 1.5 Å in length and have strengths near to, but usually less than, $100\,\text{kcal/mole}$ (418 kJ/mol). Likewise, carboncarbon double bonds are stronger (~150 kcal/mol) and shorter (~1.35 Å). Triple bonds are shorter still (C= $\text{C}\approx1.2\,\text{Å}$, ~200 kcal/mol). Bonds between carbon and either nitrogen or oxygen are somewhat shorter owing to the heteroatom's electronegativity. A few general examples are shown below and detailed data may be found in the Table 3.4.

General Trends in the Length of Common Organic Chemical Bonds

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C—C C=C C≡C	1.54 1.33 1.21	C—O C=O C—N C=N C≡N	1.43 1.20 1.47 1.28 1.15	H—C(sp³) N—H O—H C—Cl	1.12 1.03 0.97 1.76

3.14 SECTION 3

TABLE 3.4A Bond Lengths between Carbon and other Elements

The numbers in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digit.

To convert the bond length from angstroms into nanometers, multiply by 0.1; to convert angstroms into picometers, multiply by 100.

	Bond type						
	Carbon	-carbon					
Single bond Paraffinic: —C—C— In presence of —C=C— or of a In presence of —C=O bond In presence of two carbon–oxyget In presence of two carbon–carbon Aryl—C=O In presence of one carbon–carbon In presence of one carbon–introge In compounds with tendency to did In aromatic compounds In presence of carbon–carbon dou	1.541(3) 1.53(1) 1.516(5) 1.49(1) 1.426(5) 1.47(2) 1.460(3) 1.464(5) 1.44(1) 1.395(3) 1.426(5)						
$-C = C - C \equiv C -$	•						
In presence of two carbon-carbon Double bond	triple bonds: —	u≡u−c≡c−	-	1.373(4)			
Single: $-C=C-$ Conjugated with a carbon-carbon Conjugated with a carbon-oxyger Cumulative: $-C=C=C-$ or	1.337(6) 1.336(5) 1.36(1) 1.309(5)						
Triple bond Simple: −C≡C− Conjugated: −C≡C−C=C−	1.204(2) 1.206(4)						
Bond type		Bond le	ngth, Å				
	Carbon	–halogen					
	Fluorine	Chlorine	Bromine	Iodine			
Paraffinic: $R-X$ Olefinic: $-C=C-X$ Aromatic: $Ar-X$ Acetylenic: $-C\equiv C-X$	2.139(1) 2.092(5) 2.05(1) 1.99(2)						
	Bond length, Å						
	Carbon-	-hydrogen					
Paraffinic In methane In CD_4 In monosubstituted carbon: $H - C$ In disubstituted carbon: $H - C$	C—Y			1.092 1.094 1.096(5) 1.073(5)			

TABLE 3.4A Bond Lengths between Carbon and Other Elements (continued)

Bond type	Bond length, A
Carbon–hydrogen (continued)	
Paraffinic (continued)	
In trisubstituted carbon: H—C— Y	1.070(7)
Olefinic	
Simple: H—C=C— Cumultative carbon–carbon double bonds: H—C=C=C— Cumulative carbon–carbon–oxygen double bonds: H—C—C=C=O	1.083(5) 1.07(1) 1.08(1)
Aromatic	1.084(5)
Acetylenic (in C ₂ H ₂ , 1.059)	1.055(5)
In small rings	1.081(5)
In presence of a carbon triple bond: H—C=C—	1.115(4)
Carbon-nitrogen	•
Single bond	
Paraffinic: 3 covalent nitrogen: RNH ₂ , R ₂ NH, R ₃ N 4 covalent nitrogen: RNH ₃ ⁺ , R ₃ N—BX ₃ In —C—N= In aromatic compounds In conjugated heterocyclic systems (partial double bond) In —N—C=O (partial double bond)	1.472(5) 1.479(5) 1.475(10) 1.43(1) 1.353(5) 1.322(5)
Double bond: —C=N—	1.32
Triple bond (in CN radical, 1.1774): —C≡N	1.157(5)
Carbon–oxygen	
Single bond	
Paraffinic and saturated heterocyclic: —C—O—	1.426(5)
Strained, as in epoxides: $-\frac{1}{C} \frac{1}{C} \frac{1}{C} = \frac{1}{C} \frac{1}{C} \frac{1}{C} \frac{1}{C} = \frac{1}{C} \frac{1}{C} \frac{1}{C} \frac{1}{C} =$	1.435(5)
In aromatic compounds, as Ar—OH Longer bond in carboxylic acids and esters (HCOOH, 1.312) In conjugated heterocyclics, as furan	1.36(1) 1.358(5) 1.371(16)

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 TABLE 3.4A
 Bond Lengths between Carbon and Other Elements (continued)

Bond type	Bond length, Å				
Carbon–oxygen (continued)					
Double bond					
In CO $^+$ In CO In CO $_2^+$ In HCO In carbonyls In aldehydes and ketones In acyl halides: R $-$ CO $-$ X Shorter bond in carboxylic acids and esters In zwitterion forms In O $-$ C $=$ In isocyanates: RN $-$ C $=$ O In conjugated systems, as in partial triple bond: O $-$ C $-$ C $-$ C In p -quinones	1.115 1.128 1.177 1.198(8) 1.145(10) 1.215(5) 1.171(4) 1.233(5) 1.26(1) 1.160(1) 1.17(1) 1.215(5) 1.15(2)				
In metal acetylacetonates In calcite: CaCO ₃	1.28(2) 1.29(1)				
Carbon-selenium					
Single bond Paraffinic: —C—Se— In presence of fluorine, as in perfluoro compounds: —CF—Se—	1.98(2) 1.95(2)				
Double bond In Se=C=, as SeCS and SeCO In CSe radical	1.709(3) 1.67				
Carbon-silicon					
Alkyl substituent: H ₃ C—Si or H ₂ C—Si Aryl substituent: aryl—Si Electronegative substituent: R—Si—X	1.870(5) 1.843(5) 1.854(5)				
Carbon–sulfur					
Single bond Paraffinic: —C—S— In presence of fluorine, as in perfluoro-compounds: —CF—S— In heterocyclic systems: partial double bonds	1.817(5) 1.835(1) 1.718(5)				
Double bond In S=C: thiophene, S= CR_2 In sulfoxides and sulfones In presence of second carbon–carbon double bond: S= $C-C=C-$ In SC radical [in CS_2^+ , 1.554(5)]	1.71(1) 1.80(1) 1.555(1) 1.5349(2)				

TABLE 3.4A Bond Lengths between Carbon and Other Elements (*continued*)

Bond type	Bond length, Å	Bond type	Bond length, Å	
	Other elemen	ts and carbon		
C—Al	2.24(4)	C—In	2.16(4)	
C—As (paraffinic)	1.98(1)	C—Mo	2.08(4)	
С—В	1.56(1)	C—Ni	2.107(5)	
С—Ве	-Be 1.93		2.30(1)	
С—Ві	2.30	C—Pd	2.27(4)	
C—Co	1.83(2)	C—Sb (paraffinic)	2.202(16)	
C—Cr	1.92(4)	C—Sn		
C—Fe	1.84(2)	alkyl	2.143(5)	
C—Ge		electronegative		
Alkyl	1.98(3)	substituent	2.18(2)	
Aryl	1.945(5)	С—Те	1.904	
C—Hg	2.07(1)	C—Tl	2.705(5)	
in Hg(CN) ₂	1.99(2)	C—W	2.06	

 TABLE 3.4B
 Bond Lengths between Elements Other than Carbon

Elements	Bond type	Bond length, Å	Elements	Bond type	Bond length, Å
	Boron			Hydrogen (continu	ued)
В—В	B_2H_6	1.77(1)	H—Mg	MgH	1.731
B—Br	BBr_3	1.87(2)	H—Na	NaH	1.887
B—Cl	BCl_3	1.72(1)	H—Sb	H_3Sb	1.707
B—F	BF_3, R_2BF	1.29(1)	H—Se	H_2Se	1.460
В—Н	Boranes	1.21(2)	H—Sn	SnH_4	1.701
	Bridge	1.39(2)	D—Br	DBr	1.4144
B—N	Borazoles	1.42(1)	D—Cl	DCl	1.2746
В—О	$B(OH)_3$,	1.362(5)	D—I		1.6165
	$(RO)_3B$		T—Br		1.4144
			T—Cl		1.2740
	Hydrogen				
				Nitrogen	
H—Al	AlH	1.646			
H—As	AsH_3	1.519	N—Cl	NO ₂ Cl	1.79(2)
Н—Ве	BeH	1.343	N—F	NF_3	1.36(2)
H—Br	HBr	1.408	N—H	NH_4^+	1.034(3)
Н—Са	CaH	2.002		NH ₃ , RNH ₂	1.012
H—Cl	HC1	1.274		H_2NNH_2	1.038
H—F	HF	0.917		R-CO-NH ₂	0.99(3)
H—Ge	GeH_4	1.53		HN=C=S	1.013(5)
H—I	HI	1.609	N—D	ND	1.041
H-K	KH	2.244	N—N	HN_3	1.02(1)
H—Li	LiH	2.595		R_2NNH_2	1.451(5)

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TABLE 3.4B Bond Lengths between Elements Other than Carbon (*continued*)

Elements	Bond type	Bond length, Å	Elements	Bond type	Bond length, Å
	Nitrogen (continue	ed)		Phosphorus (contin	nued)
	N ₂ O	1.126(2)	Р—Н	PH ₃ , PH ₄ ⁺	1.424(5)
	N_2^+	1.116	P—I	PI_3	2.52(1)
N—O	NO ₂ Cl	1.24(1)	P—N	Single bond	1.491
	$RO-NO_2$	1.36(2)	Р—О	Single bond	1.447
	NO_2	1.188(5)		p^3 bonding	1.67
N=O	N_2O	1.186(2)		sp ³ bonding	1.54(4)
	RNO_2	1.22(1)	P—S	p^3 bonding	2.12(5)
	NO^+	1.0619		sp^3 bonding	2.08(2)
N—Si	SiN	1.572		In rings	2.20(2)
		<u> </u>	P—C	Single bond	1.562
	Oxygen			p^3 bonding	1.87(2)
О—Н	H ₂ O	0.958		Silicon	
	ROH	0.97(1)			
	OH^+	1.0289	Si—Br	SiBr ₄ , R ₃ SiBr	2.16(1)
	HOOH	0.960(5)	Si—Cl	SiCl ₄ , R ₃ SiCl	2.019(5)
	D_2O	0.9575	Si—F	SiF ₄ , R ₃ SiF	1.561(3)
	OD	0.9699		SiF ₆	1.58
0-0	но-он	1.48(1)	Si—H	SiH ₄	1.480(5)
	O_2^+	1.227		R ₃ SiH	1.476(5)
	O ₂ -	1.26(2)	Si—I	SiI ₄	2.34
	$O_2^{^2-}$	1.49(2)		R ₃ SiI	2.46(2)
	O_3	1.278(5)	Si—O	R ₃ SiOR	1.633(5)
O—Al	AlO	1.618	Si—Si	H ₃ SiSiH ₃	2.30(2)
O—As	As ₄ O ₆ (bridges)	1.79		3~-~3	
О—Ва	BaO	1.940		Sulfur	
O—Cl	ClO ₂	1.484			
	OCl ₂	1.68	S—Br	SOBr ₂	2.27(2)
O—Mg	MgO	1.749	S—Cl	-	1.585(5)
O—Os	OsO ₄	1.66	S—Ei	S ₂ Cl ₂ SOF ₂	1.585(5)
O—Pb	PbO	1.934	S—F S—Н	-	1.333
			3—п	H_2S RSH	
	Phosphorus				1.329(5) 1.345
	- moophorus		s—o	D_2S	1.343
D D.	DD.	2.22(1)	3-0	SO ₂	
P—Br	PBr ₃	2.23(1)	0 0	SOCl ₂	1.45(2)
P—Cl P—F	PCl ₃ PFCl ₂	2.00(2)	s—s	RSSR	2.05(1)
г-г	rrci ₂	1.55(3)			

The quantity $D_0(A-B)$ corresponds to the bond dissociation energy at 0 K, all species considered to be ideal gases, for a bond A-B which is broken through the reaction: Eq. $AB \rightarrow A+B$

where

$$D_0 = \Delta H f_0^{\circ}(A) + \Delta H f_0^{\circ}(B) - \Delta H f_0^{\circ}(AB)$$

 D_0 at 298 K, or ΔHf_{298} , is greater than D_0 at 0 K by an amount which lies between RT and 3/2 RT, or between 0.6 and 0.9 kcal·mol⁻¹. In polyatomic molecules this difference may be somewhat greater. It is important to note that the bond dissociation energy refers to the enthalpy change ΔHf in the dissociation process.

The numbers in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digit(s).

To convert the tabulated values (in kcal \cdot mol⁻¹) to kJ \cdot mol⁻¹, multiply by 4.184.

Source: T. L. Cottrell, *The Strengths of Chemical Bonds*, 2nd ed., Butterworth, London, 1958; B. deB. Darwent, National Standard Reference Data Series, National Bureau of Standards, no. 31, Washington, 1970; S. W. Benson, *J. Chem. Educ.*, 42: 502 (1965); and J. A. Kerr, *Chem. Rev.*, 66: 465 (1966).

TABLE 3.5 Bond Strengths (continued)

Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298}$, kcal · mol $^{-1}$	Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$
Boron			Carbon (contin	nued)	
H ₃ B—BH ₃ F ₂ B—F Bromine	133(20)	35	CH ₃ —CH ₂ CN CH ₃ —CH(CH ₃)CN CH ₃ —C(C ₆ H ₃)CN(CH ₃) C ₂ H ₅ —CH ₂ CN CH ₃ —CF ₃		73(2) 79(2) 60 76.9(17) 101.2(11)
Br—Br Br—CH ₃ Br—CH ₂ Br Br—CH ₂ Br Br—CHBr ₂ Br—CBr ₃ Br—CCl ₃ Br—CF ₂ Br—CF ₂ CF ₃ Br—CF ₂ CF ₂ CF ₃ Br—CHF ₂ Br—CI Br—F Br—CN Br—CO—C ₆ H ₅ Br—N Br—NF ₂	45.45(1) 67(2) 49(3) 51(3) 51.6(1) 67.2 68(5)	46.10(1) 68(2) 61(3) 62(4) 50(3) 52(3) 68(3) 68.7(15) 66.5(15) 69 52.3(1) 68.1 91 64	CH ₃ —CF ₃ CH ₂ F—CH ₂ F CF ₃ —CF ₃ CF ₂ =CF ₂ CF ₃ —CN CH ₂ —CO CH ₃ —CHO CH ₃ CO—CF ₃ CH ₃ CO—COCH ₃ C ₆ H ₅ CO—COCH ₅ C ₆ H ₅ CO—COC ₆ H ₅ C ₆ H ₅ CH ₂ CO—CH ₂ C ₆ H ₅ C ₆ H ₅ CH ₂ COOH (C ₆ H ₅ CH ₂) ₂ CH—COOH NC—CN CF ₃ —NF ₂ CH ₃ —NH ₂ C ₆ H ₅ CH ₂ —NH ₂	80.6	88(2) 97(2) 76(3) 120 81.9 75 73.8 67(2) 66.4 65.4 68.1 59.4 144(5) 65(3) 79(3) 72(1)

Br—NO Br—O	27.8(15) 55.3(1)	28.7(15) 56.2(1)	CH ₃ —NHC ₆ H ₅ CH ₃ —N(CH ₃)C ₆ H ₅	68 65
Carbon			$\begin{array}{c} C_{6}H_{3}CH_{2}-NHCH_{3} \\ C_{6}H_{3}CH_{2}-N(CH_{3})_{2} \end{array}$	69(1) 61(1)
HC \equiv CH H ₂ C $=$ CH ₂ CH ₃ $-$ CH ₃ CH ₃ $-$ C(CH ₃) ₂ CH ₃ CH ₃ $-$ C(CH ₃) ₃ CH ₃ $-$ C ₆ H ₅ CH ₃ $-$ Ch ₄ C ₆ H ₅ CH ₃ $-$ CH ₂ C ₆ H ₅ C ₃ H ₇ $-$ CH ₂ C ₆ H ₅ C ₃ H ₇ $-$ CH ₂ C ₆ H ₅ CH ₃ $-$ (CH $=$ CH ₂) CH ₃ $-$ (CH $=$ CH ₂) CH ₃ $-$ (CECH) (CH ₃) ₃ C $-$ C(CH ₃) ₃ (CH ₂ $-$ CH) $-$ (CH $=$ CH ₂) C ₆ H ₅ $-$ C ₆ H ₅ (HC $=$ C) $-$ (C $=$ CH) CH ₃ $-$ CC	119(5)	230(2) 163 88 69(2) 80 93 72 71 71 67(2) 29 72 117 67.5 15 100 100 150 121(5)	$\begin{array}{l} CH_{3}-(N=NCH_{3})\\ C_{2}H_{5}-(N=NC_{2}H_{5})\\ (CH_{3})_{3}C-[N=NC(CH_{3})_{3}]\\ C_{6}H_{5}CH_{2}-(N=NCH_{2}C_{6}H_{5})\\ CF_{3}-(N=NCF_{3})\\ H_{2}C=NH\\ HC\equiv N\\ CH_{3}-NO\\ C_{2}H_{5}-NO\\ C_{3}H_{7}-NO\\ (CH_{3})_{2}CH-NO\\ C_{4}H_{9}-NO\\ C_{6}H_{5}-NO\\ C_{13}C-NO\\ C_{13}C-NO\\ C_{15}C-NO\\ C_{15}C-NO\\ C_{15}C-NO\\ CC_{15}C-NO\\ $	52.5 50.0 43.5 37.6 55.2 154(5) 224 41.8(9) 42.0(13) 40.1(18) 41.0(13) 51.5(10) 51.5(10) 32 31 50.5(10) 29(3) 59(3) 62 80

TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	ΔHf_{298} , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$
Carbon (continue	d)		Chlorine (contin	ued)	
$\begin{array}{c} CH_{3} - OC_{6}H_{5} \\ CH_{3} - OCH_{2}C_{6}H_{5} \\ C_{2}H_{5} - OC_{6}H_{5} \\ C_{6}H_{5}CH_{2} - OCOCH_{3} \\ C_{6}H_{5}CH_{2} - OCOCH_{3} \\ CH_{3}CO - OCH_{3} \\ CH_{3} - O - SOCH_{3} \\ CH_{2} - CHCH_{2} - OSOCH_{3} \\ CH_{2} - CHCH_{2} - OSOCH_{3} \\ C=0 \\ H_{2}C = O \\ OC = O \\ SC = O \\ C \equiv O \\ CH_{3} - SH \\ CH_{3} - SC_{6}H_{5} \\ CH_{3} - SCH_{2}C_{6}H_{5} \\ OC - S \\ CH_{2} - CH_{3} \\ CH_{2}CH_{2} - CH_{3} \\ CH_{2}CC - CH_{3} \\ CCH_{3} - CCH_{3} \\ CCH_{4} - CCH_{4} \\ CCH_{4} - CCH_{5} \\ CCH_{5} - CCH_{5} \\ CCH_{5}$	256.2(1) 125.7(1) 148 71(3) 72.9	91 67 51 69 97 67 50 53 257.3(1) 175 127.2(1) 150 257 73(3) 68(2) 59(2) 74.2 96 25.5 51 32 27.5	Cl—COC ₆ H ₅ Cl—Cl ⁺ Cl—Cl Cl—Cl Cl—ClO O ₃ Cl—ClO ₄ Cl—F O ₃ Cl—F Cl—N Cl—NCl Cl—NCl Cl—NP ₂ Cl—NH ₂ Cl—NO Cl—NO ₂ Cl—O OCl—O OCl—O OCl—O The Cl—O Cl—SiCl ₃ Cl—CH ₃ The Cl—Cl Fluorine	57.3(1) 33.3(10) 59.5(5) 37.0(15) 33(1) 64(1) 58(3)	74(3) 94 58 61 62 67 91 ca 32 60(6) 38.0(15) 34(1) 48(1) 111 51 94

CH_3 CH_3 CH_3 CH_3 CCH_3 $CCCH_3$ CCH_3 CCH_3 CCH_3 CCH_3 CCH_3 CCH_3 $CCCH_3$ CCH_3 CCH_3 CCH_3 CCH_3 CCH_3 CCH_3 $CCCCCH_3$ CCH_3 $CCCCCCCC$ $CCCCCCCC$ $CCCCCCCC$ $CCCCCCCC$		35 11.5 20 12 7 30 11 -20 46 119 162 223		37(1) 64(3) 18.4 71(10) 75(5) 57(2) 55.2(10) 46(5) > 60	116 106(5) 110(6) 117(6) 125(4) 119 72(10) 76(5) 58(2) 56.3(10)
Chlorine			CH ₃ —Ga(CH ₃) ₃	59.5	
Cl—C Cl—CH ₃	80(10)	80.8 81(5) 78.5 74(3) 70(5) 86.1(8) 73(2) 76(2) 82.7(17) 84 105 78.5 83.5	Hydrogen		
$CI - C(CH_3)_3$ $CI - CH_2CI$ $CI - CCI_3$ $CI - CF_3$ $CI - CCI_2F$ $CI - CF_2CI$ $CI - CF_2CF_3$ $CI - (CH = CH_2)$ CI - CN CI - COCI $CI - COCH_3$			H-Br H-C H-CH $H-CH_2$ $H-CH_3$ $D-CD_3$ $H-(C \equiv CH)$ $H-(C = CH_2)$ $H-CH_2CH_3$ $H-CH_2C \equiv CH$ $H-CH_2C \equiv CH$	86.6(1) 80 112.3(1) 102(2) 104.92(5)	87.5(1) 81.0(5) 108(6) 113(1) 103(2) 125(1) 102 98(1) 93.9(12) 85

Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$	Bond	D_0° , kcal · mol ⁻¹	$\Delta Hf_{298},$ kcal \cdot mol $^{-1}$
Hydrogen (continued)			Hydrogen (continued)		
H—cyclopropyl H—CH ₂ CH ₂ CH ₃ H—CH(CH ₃) ₂ H—cyclobutyl H—CH ₂ CH(CH ₃) ₂ H—CH(CH ₃)CH ₂ CH ₃ H—C(CH ₃) ₃ H—C(CH ₂) H—CH CH=CH ₂ H—CH CH=CH ₂ H—CH CH ₂ C CH ₂ H—CH ₂ CH ₃ H—CH CH ₂ CH ₃ H—CH CH ₂ CH ₃ H—CH CH ₂ CH ₃ H—CH ₂ Ch ₃ CH=CH ₃ H—CH ₂ Ch ₃ CH=CH ₃ H—CH ₂ Ch ₃ CH=CH ₃		101(3) 98(2) 94.5 95(3) 86 95(1) 91 81(1) 82(1) 99(1) 79 94.5(10) 100(1) 103 85(1)	H—CI H—CO H—CHO H—CHO H—COOH H—COCH ₃ H—COCH ₂ CH ₃ H—COCF ₃ H—F H—H H—D D—D H—I H—N H—NH H—NH ₂ H—NHCH ₃ H—N(CH ₃) ₂ H—N(CH ₃) ₂ H—N(CH ₃) ₂ H—N(CH ₃) ₆ H ₅ H—NF ₂ H—NF ₂ H—NF ₂	135(1) 103.25 104.07(1) 105.05(1) 70.4(1) 85(2) 89(2) 103(2)	30(2) 87(1) 90 87(1) 87(1) 92(1) 87(1) 91(2) 135.8 104.19 105.00 105.96 71.3(1) 85(2) 90(2) 104(2) 103(2) 95(2) 80(3) 74(3) 76(3) 85

$H-C(C_6H_5)_3$		75	H—NO		< 49
			H—O	101.3(5)	102.3(5)
H—		74	Н—ОН	118.0(2)	119.2(2)
" _/			H—OCH ₃		104.4(10
			H—OCH ₂ CH ₃		104.2
H—cyclohexyl		95.5(10)	$H - OC(CH_3)_3$		105(1)
H—cycloheptyl		92.5(10)	$H - OCH_2C(CH_3)_3$		102.3(15
H—norbornyl		97(3)	$H-OC_6H_5$		88(5)
H—CH ₂ Br	97(5)		H—ONO		78.3(5)
H—CHBr ₂		104	H—ONO ₂		101.2(5)
H—CBr ₃	88(2)	90(2)	H—OOH	88.5(20)	89.5(20)
H—CH ₂ Cl		101	H—OOCCH ₃		112(4)
H—CHCl ₂		99.0	H—OOCCH ₂ CH ₃		110(4)
H—CCl ₃	89(3)	90(3)	H—OOCC ₃ H ₇		103(4)
H—CCl ₂ CHCl ₂		94(2)	H—SH	90(1)	91(1)
H—CCl ₂ CCl ₃		95(2)	H—SCH ₃		ca 88
H—CH ₂ F		101(2)	H—SiH ₃		94(3)
H—CHF ₂		101(2)	H—Si(CH ₃) ₃		90(3)
H—CF ₃	105(3)	106(3)	H—SiCl ₃		91.3(14)
H—CF ₂ Cl		104(1)	ĊH ₂ —H		106
H—CH ₂ CF ₃		106.7(11)	ĊН—Н		106
H—CF ₂ CH ₃		99.5(1)	Ċ—Н		81
H—CF ₂ CF ₃		103.1(15)	ĊH ₂ CH ₂ —H		39
H—CF ₂ CF ₂ CF ₃		104(2)	ÖCH ₂ —Н		22
H—CH ₂ I		103(2)	ĊО—Н		19
H—CHI ₂		103(2)	ĊНСН—Н		43
H—CN	127(5)	129(5)	∥ H—Ò		102
H—CH ₂ CN		ca 93	H—OÒ		47
H—CH(CH ₃)CN		90(2)	H—OĊH ₂		31
H — $C(CH_3)_2CN$		87(2)	H—OOĊ		31
H — CH_2NH_2		95(2)	ĊН—Н		ca 125
H — $CH_2Si(CH_3)_3$		99(1)	ĊOCH ₂ —H		43.5
H—CH ₂ COCH ₃		98.3(18)			

TABLE 3.5 Bond Strengths (*continued*)

Bond	$D_0^{\circ},$ kcal \cdot mol $^{-1}$	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$	Bond	D_0° , kcal \cdot mol $^{-1}$	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$
Hydrogen (continu	ed)		Nitrogen		
ĊH ₂ CO—H		36	N—N F ₂ N—NF ₂	225.07(1) 20(1)	225.96(1) 21(1)
Н		40	H ₂ N—NH ₂ H ₂ N—NHCH ₃ H ₂ N—N(CH ₃),		71(2) 65 63
Н		47.5	H ₂ N — NHC ₆ H ₅ HN — N ₂ ON — N	113.5(10)	51 9(1) 114.9(10)
Н		24	ON—NO ₂ O ₂ N—NO ₂	8.4(2) 12.7(5)	9.5(2) 13.7(5)
C+—H		85	NN—O		40
CH ₃ +—H		30 29	ON—O HN—NH		73 109(10)
CH ₃ CH ₂ ⁺ —H CH ₂ CH ₃ ⁺ —H		79	HN=O		115
H—H ⁺		62	N≡N		226
			N—N ⁺		200
Iodine			N—NO ⁺		155
	T		NN—O ⁺		56
I—Br	41.9(1)	42.5(1)	ON ⁺ —O		56
I—CH ₃ I—CH ₂ CH ₃	54(3)	55.5(30) 53.5	Osmium		
I—CH ₂ CH ₃ I—CH(CH ₃) ₂		53.5	O ₃ Os—O		72(5)
$I-C(CH_3)_2$		49.5	Oxygen		
I—CH ₂ CF ₃ I—CF ₂ CH ₃		56(1) 52(1)	HO—CH ₃ HO—(CH=CH ₂)	88.5(30)	90(3) 87

$I-CF_{2}CF_{3}$ $I-C_{3}F_{7}$ $I-(CH=CHCH_{3})$ $I-CH_{3}^{+}$ $I-C_{6}H_{5}$ $I-C_{6}F_{5}$ $I-C1$ $I-COCH_{3}$ $I-CN$ $I-F$ $I^{+}-H$ $I-I$ $I-I^{+}$ $I-NO$ $I-NO_{2}$ Lead	49.7(1) 66.4(10) 35.60(1)	51(1) 50(1) 41 62 64(1) 66 50.5(1) 52.5 73(1) 67(1) 70 36.15 61 17(1) 18(1)	HO—CH ₂ CH=CH ₂ HO—C ₆ H ₅ HO—CH ₂ C ₆ H ₅ HO—CHO HO—COCH ₃ HO—COCH ₂ CH ₃ HO—CI HO—I HO—NCH ₃ HO—OC(CH ₃) ₃ O—O HO—OH CF ₃ O—OCF ₃ C ₂ H ₅ O—OC ₂ H ₅ C ₃ H ₇ O—OC ₃ H ₇ O—OF O—O ₅ CIF	117.97(10) 49.5(5)	109 103 77 96(3) 108(5) 43 60(3) 56(3) 50 46(2) 119.11 51.1(5) 46 37.6(2) 38 37
CH ₃ —Pb(CH ₃) ₃		49.4(10)	FO—OF O—PBr ₃		62(20) 119(5)
Lithium			0=PCl ₃ 0=PF ₃ 0-O ⁺		122(5) 130(5) 168
Li—H	58		HO—CH ₃		67
Mercury			Phosphorus		
Hg—Br CH ₃ —HgCH ₃ C ₂ H ₅ —HgC ₂ H ₅ C ₃ H ₇ —HgC ₃ H ₇ (CH ₃) ₂ CH—HgCH(CH ₃) ₂ C ₆ H ₅ —HgC ₆ H ₅	16.4(10)	17.4(10) 57.5 43.7(10) 47.1 40.7 68	P—Br P—Cl P—F P—H P—O P—P P=S	141.5(10) 115(2) 82	63.7 78.5 117 79(1) 142.3(10) 116(2)

TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298}$, kcal \cdot mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	$\Delta H f_{298},$ kcal \cdot mol $^{-1}$		
Ruthenium			Sulfur				
O—RuO ₃	O—RuO ₃ 104			16	61		
Selenium			O ₂ S—F S—N S—O	115 123.6(20)			
Se—Cl Se—F Se—O Se—Se	81(23) 65	58 68	OS — O O ₂ S — O S — S HS — SH S — Te	130.8(20) 81.9(10) 101.5(15)	83.2(10) 102.5(15) 65(5)		
Silicon			HS ⁺ —H HS—H ⁺		104 161		
Si—Br Si—Cl	69(14) 76(12)	135 56 42 81(4)	OS—O ⁺ 155				
Si—F Si—H Si—I Si—N Si—O Si—S Si—Se Si—Se Si—Si H ₃ Si—SiH ₃	74(6) ca 104 185(7) 147(3) 134(6)		BrSn—Br Br ₃ Sn—Br C ₂ H ₅ Sn—(C ₂ H ₅) ₃ Sn—Cl Sn—H Sn—I Sn—O Sn—S	130(5) 111(5)	78 65 ca 57 76 61.0(7) 65 131(5) 112(5)		
$(CH_3)_3Si-Si(CH_3)_3$ $(C_6H_5)_3Si-Si(C_6H_5)_3$		81 88(7)	Xenon				
$(C_6\Pi_5/3)\Pi = SI(C_6\Pi_5/3)$ Si—Te	122(9)	00(7)	Xe—F		31(1)		

Sodium		Zinc			
Na—H Na—K Na—Na Na—OH	47 14.3 17.3	91(3)	$Zn-H$ $C_2H_5Zn-C_2H_5$	19.6(5)	ca 48

3.30 SECTION 3

BOND AND GROUP DIPOLE MOMENTS

All bonds between equal atoms are given zero values. Because of their symmetry, methane and ethane molecules are nonpolar. The principle of bond moments thus requires that the CH_3 group moment equal one H—C moment. Hence the substitution of any aliphatic H by CH_3 does not alter the dipole moment, and all saturated hydrocarbons have zero moments as long as the tetrahedral angles are maintained.

The group moment always includes the C—X bond. When the group is attached to an aromatic system, the moment contains the contributions through resonance of those polar structures postulated as arising through charge shifts around the ring.

All values for bond and group dipole moments in Tables 3.6 and 3.7 were obtained in benzene solution.

TABLE 3.6 Bond Dipole Moments

Bond	Moment, D*	Bond	Moment, D*
H—C		Se—C	0.7
Aliphatic	0.3	Si—C	1.2
Aromatic	0.0	Si—H	1.0
C-C	0.0	Si—N	1.55
C≡C	0.0	H—Sb	-0.08
C-0		G—As	-0.10
Ether, aliphatic	0.74	H—P	0.36
Alcohol, aliphatic	0.7	H—I	0.38
C=0		H—Br	0.78
Aliphatic	2.4	H—Cl	1.08
Aromatic	2.65	H—F	1.94
О—Н	1.51	С—Те	0.6
C—S	0.9	N—F	0.17
C=S	2.0	P—I	0.3
S—H	0.65	P—Br	0.36
S—O	(0.2)	P—Cl	0.81
S=0	, ,	As—I	0.78
Aliphatic	2.8	As—Br	1.27
Aromatic	3.3	As—Cl	1.64
C-N, aliphatic	0.45	As—F	2.03
C=N	1.4	Sb—I	0.8
C≡N (nitrile)	3.6	Sb—Br	1.9
NC (isonitrile)	3.0	Sb—Cl	2.6
N—H	1.31	S—Cl	0.7
N—O	0.3	Cl—O	0.7
N=0	2.0	I—Br	1.2
N : lone pair on sp^3N	1.0	I—Cl	1
C—P, aliphatic	0.8	Br—Cl	0.57
P-0	(0.3)	Br—F	1.3
P=0	2.7	Cl—F	0.88
P—S	0.5	Li—C	1.4
P=S	2.9	K—Cl	10.6
B—C, aliphatic	0.7	K—F	7.3
В—О	0.25		

TABLE 3.6 Bond Dipole Moments (*continued*)

Bond	Moment, D*	Bond	Moment, D*
Cs—Cl Cs—F	10.5	Dative (coordination	on) bonds (continued)
_s—r	7.9	$P \rightarrow O$	2.9
Dative (coo	ordination) bonds	$S \rightarrow O$	3.0
		$As \rightarrow O$	4.2
$N \rightarrow B$	2.6	$Se \rightarrow O$	3.1
$O \rightarrow B$	3.6	$Te \rightarrow O$	2.3
$S \rightarrow B$	3.8	$P \rightarrow S$	3.1
$P \rightarrow B$	4.4	$P \rightarrow Se$	3.2
$N \rightarrow O$	4.3	$Sb \rightarrow S$	4.5

^{*}To convert debye units D into coulomb-meters, multiply by 3.33564×10^{-30} .

TABLE 3.7 Group Dipole Moments

	Mon	nent, D*
Group	Aromatic C—X	Aliphatic C—X
C—CH ₃	0.37	0.0
$C-C_2H_5$	0.37	0.0
$C-C(CH_3)_3$	0.5	0.0
$C-CH=CH_2$	< 0.4	0.6
C—C≡CH	0.7	0.9
C—F	1.47	1.79
C—Cl	1.59	1.87
C—Br	1.57	1.82
C—I	1.40	1.65
C—CH ₂ F	1.77(g)	
C—CF ₃	2.54	2.32
C—CH ₂ Cl	1.85	1.95
C—CHCl ₂	2.04	1.94
C—CCl ₃	2.11	1.57
C—CH ₂ Br	1.86	1.96
$C-C\equiv N$	4.05	3.4
C—NC	3.5	3.5
C-CH ₂ CN	1.86	2.0
C-C=0	2.65	2.4
C—CHO	2.96	2.49
C—COOH	1.64	1.63
C—CO—CH ₃	2.96	2.75
C—CO—OCH ₃	1.83	1.75
$C-CO-OC_2H_5$	1.9	1.8
С—ОН	1.6	1.7
C—OCH ₃	1.28	1.28
C—OCF ₃	2.36	

3.32 SECTION 3

TABLE 3.7 Group Dipole Moments (*continued*)

	Mon	nent, D*
Group	Aromatic C—X	Aliphatic C—X
C—OCOCH ₃	1.69	
$C-OC_6H_5$	1.16	1.16
C—CH ₂ OH	1.68	1.68
C—NH ₂	1.53	1.46
C—NHCH ₃	1.71	
$C-N(CH_3)_2$	1.58	0.86
C—NHCOCH ₃	3.69	
$C - N(C_6H_5)_2$	(0.3)	-0.3
C—NCO	2.32	2.8
$C-N_3$	1.44	
C-NO	3.09	
C—NO ₂	4.01	2.70
C—CH ₂ NO ₂	3.3	3.4
C—SH	1.22	1.55
C—SCH ₃	1.34	1.40
C—SCF ₃	2.50	
C—SCN	3.59	3.6
C—NCS	2.9	3.3
$C-SC_6H_5$	1.51	1.5
C—SF ₅	3.4	
C—SOCF ₃	3.88	
$(C-)_2SO_2$	5.05	4.53
$(C-)_2SO_2CH_3$	4.73	
$(C-)_2SO_2CF_3$	4.32	
C—SeH	1.08	
C—SeCH ₃	1.31	1.32
C — $Si(CH_3)_3$	0.44	0.4

^{*}To convert debye units D into coulomb-meters, multiply by 3.33564×10^{-30} .

SECTION 4

PHYSICAL PROPERTIES

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4.2 SECTION 4

SOLUBILITIES

TABLE 4.1 Solubility of Gases in Water

Explanation of the column headings

 α , Volume of gas in milliliters (mL). The column or line entry headed " α " gives the volume of gas (in milliliters) at standard conditions (0°C and 760 mm or 101.325 kN·m⁻²) dissolved in 1 mL of water at the temperature stated (in degrees Celsius) and when the pressure of the gas without the water vapor is 760 mm.

A, Volume of gas in milliliters (mL). The line entry "A" indicates the same quantity as " α " except that the gas itself is at the uniform pressure of 760 mm when in equilibrium with water.

1, Volume of gas in milliliters (mL). The column headed "1" gives the volume of the gas (in milliliters) dissolved in 1 mL of water when the pressure of the gas plus that of the water vapor is 760 mm.

q, Weight of the gas in grams (g). The column headed "q" gives the weight of gas (in grams) dissolved in 100 g of water when the pressure of the gas plus that of the water vapor is 760 mm

	Ace	etylene	Air*		Am	monia	Bromine	
Temp. °C	α	q	$\alpha(\times 10^3)$	% oxygen in air	α	q	α	q
0	1.73	0.200	29.18	34.91	1130	89.5	60.5	42.9
1	1.68	0.194	28.42	34.87	—	_		_
2	1.63	0.188	27.69	34.82	_	_	54.1	38.3
3 4	1.58	0.182	26.99	34.78		70.6	48.3	24.2
5	1.53 1.49	0.176 0.171	26.32 25.68	34.74 34.69	1047	79.6	48.3	34.2
6	1.49	0.171	25.06	34.65		_	43.3	30.6
7	1.43	0.167	24.47	34.60	_	_	45.5	30.0
8	1.37	0.162	23.90	34.56	947	72.0	38.9	27.5
9	1.34	0.154	23.36	34.52) /	72.0	30.9	
10	1.31	0.150	22.84	34.47	870	68.4	35.1	24.8
11	1.27	0.146	22.34	34.43		—		
12	1.24	0.142	21.87	34.38	857	65.1	31.5	22.2
13	1.21	0.138	21.41	34.34	837	63.6		_
14	1.18	0.135	20.97	34.30	_	_	28.4	20.0
15	1.15	0.131	20.55	34.25	770	_	_	_
16	1.13	0.129	20.14	34.21	775	58.7	25.7	18.0
17	1.10	0.125	19.75	34.17	_	_	_	_
18	1.08	0.123	19.38	34.12	—		23.4	16.4
19	1.05	0.119	19.02	34.08	l —	_	_	_
20	1.03	0.117	18.68	34.03	680	52.9	21.3	14.9
21	1.01	0.115	18.34	33.99	_	_	_	_
22	0.99	0.112	18.01	33.95	_	_	19.4	13.5
23	0.97	0.110	17.69	33.90				
24	0.95	0.107	17.38	33.86	639	48.2	17.7	12.3
25	0.93	0.105	17.08	33.82	—	_		
26 27	0.91	0.102	16.79	33.77	_	_	16.3	11.3
	0.89	0.100	16.50 16.21	33.73	 586	44.0	15.0	10.2
28 29	0.87 0.85	0.098 0.095	15.92	33.68 33.64	386	44.0	15.0	10.3
30	0.83	0.093	15.64	33.60	530	41.0	13.8	9.5
35	0.04	0.054	13.04	33.00	330	41.0	13.6	9.5
40		<u> </u>	14.18	_	400	31.6	9.4	6.3
45	_		——————————————————————————————————————			J1.0	JT	
50		_	12.97	_	290	23.5	6.5	4.1
60	l _		12.16	_	200	16.8	4.9	2.9
70	_			_		11.1	3.8	1.9
80	_		11.26	_	l _	6.5	3.0	1.2
90	_			_	l <u> </u>	3.0	_	
100	_	_	11.05	_	l —	0.0	_	

^{*}Free from NH₃ and CO₂; total pressure of air + water vapor is 760 mm.

 TABLE 4.1
 Solubility of Gases in Water (continued)

Temp.	Carbon dioxide		Carbon monoxide		Chle	Chlorine		Ethane		ylene	Hydrogen	
°C	α	q	α	q	1	q	α	q	α	q	α	q
0 1 2 3 4	1.713 1.646 1.584 1.527 1.473	0.334 6 0.321 3 0.309 1 0.297 8 0.287 1	0.035 37 0.034 55 0.033 75 0.032 97 0.032 22	0.004 397 0.004 293 0.004 191 0.004 092 0.003 996	_ _ _ _	_ _ _ _	0.098 74 0.094 76 0.090 93 0.087 25 0.083 72	0.013 17 0.012 63 0.012 12 0.011 62 0.011 14	0.226 0.219 0.211 0.204 0.197	0.028 1 0.027 2 0.026 2 0.025 3 0.024 4	0.021 48 0.021 26 0.021 05 0.020 84 0.020 64	0.000 192 2 0.000 190 1 0.000 188 1 0.000 186 2 0.000 184 3
5 6 7 8 9	1.424 1.377 1.331 1.282 1.237	0.277 4 0.268 1 0.258 9 0.249 2 0.240 3	0.031 49 0.030 78 0.030 09 0.029 42 0.028 78	0.003 903 0.003 813 0.003 725 0.003 640 0.003 559	_ _ _ _	_ _ _ _	0.080 33 0.077 09 0.074 00 0.071 06 0.068 26	0.010 69 0.010 25 0.009 83 0.009 43 0.009 06	0.191 0.184 0.178 0.173 0.167	0.023 7 0.022 8 0.022 0 0.021 4 0.020 7	0.020 44 0.020 25 0.020 07 0.019 89 0.019 72	0.000 182 4 0.000 180 6 0.000 178 9 0.000 177 2 0.000 175 6
10 11 12 13 14	1.194 1.154 1.117 1.083 1.050	0.231 8 0.223 9 0.216 5 0.209 8 0.203 2	0.028 16 0.027 57 0.027 01 0.026 46 0.025 93	0.003 479 0.003 405 0.003 332 0.003 261 0.003 194	3.148 3.047 2.950 2.856 2.767	0.997 2 0.965 4 0.934 6 0.905 0 0.876 8	0.065 61 0.063 28 0.061 06 0.058 94 0.056 94	0.008 70 0.008 38 0.008 08 0.007 80 0.007 53	0.162 0.157 0.152 0.148 0.143	0.020 0 0.019 4 0.018 8 0.018 3 0.017 6	0.019 55 0.019 40 0.019 25 0.019 11 0.018 97	0.000 174 0 0.000 172 5 0.000 171 0 0.000 169 6 0.000 168 2
15 16 17 18 19	1.019 0.985 0.956 0.928 0.902	0.197 0 0.190 3 0.184 5 0.178 9 0.173 7	0.025 43 0.024 94 0.024 48 0.024 02 0.023 60	0.003 130 0.003 066 0.003 007 0.002 947 0.002 891	2.680 2.597 2.517 2.440 2.368	0.849 5 0.823 2 0.797 9 0.773 8 0.751 0	0.055 04 0.053 26 0.051 59 0.050 03 0.048 58	0.007 27 0.007 03 0.006 80 0.006 59 0.006 39	0.139 0.136 0.132 0.129 0.125	0.017 1 0.016 7 0.016 2 0.015 8 0.015 3	0.018 83 0.018 69 0.018 56 0.018 44 0.018 31	0.000 166 8 0.000 165 4 0.000 164 1 0.000 162 8 0.000 161 6
20 21 22 23 24	0.878 0.854 0.829 0.804 0.781	0.168 8 0.164 0 0.159 0 0.154 0 0.149 3	0.023 19 0.022 81 0.022 44 0.022 08 0.021 74	0.002 838 0.002 789 0.002 739 0.002 691 0.002 646	2.299 2.238 2.180 2.123 2.070	0.729 3 0.710 0 0.691 8 0.673 9 0.657 2	0.047 24 0.045 89 0.044 59 0.043 35 0.042 17	0.006 20 0.006 02 0.005 84 0.005 67 0.005 51	0.122 0.119 0.116 0.114 0.111	0.014 9 0.014 6 0.014 2 0.013 9 0.013 5	0.018 19 0.018 05 0.017 92 0.017 79 0.017 66	0.000 160 3 0.000 158 8 0.000 157 5 0.000 156 1 0.000 154 8

 TABLE 4.1
 Solubility of Gases in Water (continued)

Томи	Carbo	n dioxide	Carbon 1	monoxide	Chle	orine	Eth	nane	Eth	ylene	Hydro	gen
Temp. °C	α	q	α	q	1	q	α	q	α	q	α	q
25 26 27 28 29 30 35 40 45 50	0.759 0.738 0.718 0.699 0.682 0.665 0.592 0.530 0.479 0.436	0.144 9 0.140 6 0.136 6 0.132 7 0.129 2 0.125 7 0.110 5 0.097 3 0.086 0 0.076 1	0.021 42 0.021 10 0.020 80 0.020 51 0.020 24 0.019 98 0.018 77 0.017 75 0.016 90 0.016 15	0.002 603 0.002 560 0.002 519 0.002 479 0.002 442 0.002 405 0.002 231 0.002 075 0.001 933 0.001 797	2.019 1.970 1.923 1.880 1.839 1.799 1.602 1.438 1.322 1.225	0.641 3 0.625 9 0.611 2 0.597 5 0.584 7 0.572 3 0.510 4 0.459 0 0.422 8 0.392 5	0.041 04 0.039 97 0.038 95 0.037 99 0.037 09 0.036 24 0.032 30 0.029 15 0.026 60 0.024 59	0.005 35 0.005 20 0.005 06 0.004 93 0.004 80 0.004 68 0.004 12 0.003 66 0.003 27 0.002 94	0.108 0.106 0.104 0.102 0.100 0.098	0.013 1 0.012 9 0.012 6 0.012 3 0.012 1 0.011 8	0.017 54 0.017 42 0.017 31 0.017 20 0.017 09 0.016 99 0.016 66 0.016 44 0.016 24 0.016 08	0.000 153 5 0.000 152 2 0.000 150 9 0.000 149 6 0.000 148 4 0.000 147 4 0.000 142 5 0.000 134 1 0.000 128 7
60 70 80 90 100	0.359 — — — —	0.057 6 — — — —	0.014 88 0.014 40 0.014 30 0.014 2 0.014 1	0.001 797 0.001 522 0.001 276 0.000 980 0.000 57 0.000 00	1.023 0.862 0.683 0.39 0.00	0.329 5 0.279 3 0.222 7 0.127 0.000	0.024 39 0.021 77 0.019 48 0.018 26 0.017 6 0.017 2	0.002 94 0.002 39 0.001 85 0.001 34 0.000 8 0.000 0			0.016 00 0.016 0 0.016 0 0.016 0 0.016 0	0.000 128 7 0.000 117 8 0.000 102 0.000 079 0.000 046 0.000 000

 TABLE 4.1
 Solubility of Gases in Water (continued)

	Hydrog	gen sulfide	Me	ethane	Nitrio	oxide	Nit	trogen*	Оху	gen	Sulfur	dioxide
Temp. °C	α	q	α	q	α	q	α	q	α	q	1	q
0 1 2 3	4.670 4.522 4.379 4.241 4.107	0.706 6 0.683 9 0.661 9 0.640 7	0.055 63 0.054 01 0.052 44 0.050 93 0.049 46	0.003 959 0.003 842 0.003 728 0.003 619	0.073 81 0.071 84 0.069 93 0.068 09	0.009 833 0.009 564 0.009 305 0.009 057	0.023 54 0.022 97 0.022 41 0.021 87	0.002 942 0.002 869 0.002 798 0.002 730	0.048 89 0.047 58 0.046 33 0.045 12	0.006 945 0.006 756 0.006 574 0.006 400	79.789 77.210 74.691 72.230	22.83 22.09 21.37 20.66
4 5 6 7 8 9	3.977 3.852 3.732 3.616 3.505	0.620 1 0.600 1 0.580 9 0.562 4 0.544 6 0.527 6	0.049 46 0.048 05 0.046 69 0.045 39 0.044 13 0.042 92	0.003 513 0.003 410 0.003 312 0.003 217 0.003 127 0.003 039	0.066 32 0.064 61 0.062 98 0.061 40 0.059 90 0.058 46	0.008 816 0.008 584 0.008 361 0.008 147 0.007 943 0.007 747	0.021 35 0.020 86 0.020 37 0.019 90 0.019 45 0.019 02	0.002 663 0.002 600 0.002 537 0.002 477 0.002 419 0.002 365	0.043 97 0.042 87 0.041 80 0.040 80 0.039 83 0.038 91	0.006 232 0.006 072 0.005 918 0.005 773 0.005 632 0.005 498	69.828 67.485 65.200 62.973 60.805 58.697	19.98 19.31 18.65 18.02 17.40 16.80
10 11 12 13 14	3.399 3.300 3.206 3.115 3.028	0.511 2 0.496 0 0.481 4 0.467 4 0.454 0	0.041 77 0.040 72 0.039 70 0.038 72 0.037 79	0.002 955 0.002 879 0.002 805 0.002 733 0.002 665	0.057 09 0.055 87 0.05470 0.053 57 0.052 50	0.007 560 0.007 393 0.007 233 0.007 078 0.006 930	0.018 61 0.018 23 0.017 86 0.017 50 0.017 17	0.002 312 0.002 263 0.002 216 0.002 170 0.002 126	0.038 02 0.037 18 0.036 37 0.035 59 0.034 86	0.005 368 0.005 246 0.005 128 0.005 014 0.004 906	56.647 54.655 52.723 50.849 49.033	16.21 15.64 15.09 14.56 14.04
15 16 17 18 19	2.945 2.865 2.789 2.717 2.647	0.441 1 0.428 7 0.416 9 0.405 6 0.394 8	0.036 90 0.036 06 0.035 25 0.034 48 0.033 76	0.002 599 0.002 538 0.002 478 0.002 422 0.002 369	0.051 47 0.050 49 0.049 56 0.048 68 0.047 85	0.006 788 0.006 652 0.006 524 0.006 400 0.006 283	0.016 85 0.016 54 0.016 25 0.014 97 0.015 70	0.002 085 0.002 045 0.002 006 0.001 970 0.001 935	0.034 15 0.033 48 0.032 83 0.032 20 0.031 61	0.004 802 0.004 703 0.004 606 0.004 514 0.004 426	47.276 45.578 43.939 42.360 40.838	13.54 13.05 12.59 12.14 11.70

Temp.	Hydrog	en sulfide	Me	ethane	Nitrio	oxide	Nitro	ogen*	Oxy	/gen	Sulfur	dioxide
°C	α	q	α	q	α	q	α	q	1	q	α	q
20 21 22 23	2.582 2.517 2.456 2.396	0.384 6 0.374 5 0.364 8 0.355 4	0.033 08 0.032 43 0.031 80 0.031 19	0.002 319 0.002 270 0.002 222 0.002 177	0.047 06 0.046 25 0.045 45 0.044 69	0.006 173 0.006 059 0.005 947 0.005 838	0.015 45 0.015 22 0.014 98 0.014 75	0.001 901 0.001 869 0.001 838 0.001 809	0 031 02 0.030 44 0.029 88 0.029 34	0.004 339 0.004 252 0.004 169 0.004 087	39.374 37.970 36.617 35.302	11.28 10.88 10.50 10.12
24 25 26 27 28 29	2.338 2.282 2.229 2.177 2.128 2.081	0.346 3 0.337 5 0.329 0 0.320 8 0.313 0 0.305 5	0.030 61 0.030 06 0.029 52 0.029 01 0.028 52 0.028 06	0.002 133 0.002 091 0.002 050 0.002 011 0.001 974 0.001 938	0.043 95 0.043 23 0.042 54 0.041 88 0.041 24 0.040 63	0.005 733 0.005 630 0.005 530 0.005 435 0.005 342 0.005 252	0.014 54 0.014 34 0.014 13 0.013 94 0.013 76 0.013 58	0.001 780 0.001 751 0.001 724 0.001 698 0.001 672 0.001 647	0.028 81 0.028 31 0.027 83 0.027 36 0.026 91 0.026 49	0.004 007 0.003 931 0.003 857 0.003 787 0.003 718 0.003 651	34.026 32.786 31.584 30.422 29.314 28.210	9.76 9.41 9.06 8.73 8.42 8.10
30 35 40 45 50	2.037 1.831 1.660 1.516 1.392	0.298 3 0.264 8 0.236 1 0.211 0 0.188 3	0.027 62 0.025 46 0.023 69 0.022 38 0.021 34	0.001 904 0.001 733 0.001 586 0.001 466 0.001 359	0.040 04 0 037 34 0.035 07 0.033 11 0.031 52	0.005 165 0.004 757 0.004 394 0.0040 59 0.003 758	0.013 42 0.012 56 0.011 84 0.011 30 0.010 88	0.001 624 0.001 501 0.001 391 0.001 300 0.001 216	0.026 08 0.024 40 0.023 06 0.021 87 0.020 90	0.003 588 0.003 315 0.003 082 0.002 858 0.002 657	27.161 22.489 18.766 —	7.80 6.47 5.41 —
60 70 80 90 100	1.190 1.022 0.917 0.84 0.81	0.148 0 0.1101 0.076 5 0.041 0.000	0.019 54 0.018 25 0.017 70 0.017 35 0.017 0	0.001 144 0.000 926 0.000 695 0.000 40 0.000 00	0.029 54 0.028 10 0.027 00 0.026 5 0.026 3	0.003 237 0.002 668 0.001 984 0.001 13 0.000 00	0.010 23 0.009 77 0.009 58 0.009 5 0.009 5	0.001 052 0.000 851 0.000 660 0.000 38 0.000 00	0.019 46 0.018 33 0.017 61 0.017 2 0.017 0	0.002 274 0.001 856 0.001 381 0.000 79 0.000 00		_ _ _

^{*}Atmospheric nitrogen containing 98.815% N_2 by volume + 1.185% inert gases.

 TABLE 4.1
 Solubility of Gases in Water (continued)

Substance		0°	10°	20°	30°	40°	60°	80°
Argon Helium Hydrogen bromide Hydrogen chloride Krypton Neon Nitrous oxide Ozone Radon Xenon	$\begin{array}{c} \alpha \\ A \\ 1 \\ \alpha \\ \alpha \\ A \\ A \\ g \cdot L^{-1} \\ \alpha \\ \alpha \end{array}$	0.052 8 0.009 8 612 512 0.110 5 0.039 4 0.510 0.242	0.041 3 0.009 11 582 475 0.081 0 0.011 79° 0.88 0.029 912° 0.326 0.174	0.033 7 0.008 6 442 0.062 6 0.010 6 0.63 0.021 0 ¹⁹⁹ 0.222 0.123	0.028 8 0.008 39 533 ^{25°} 412 0.051 1 0.010 0 0.0139 ^{27°} 0.162 0.098	0.025 1 0.008 41 385 0.043 3 0.009 48 ^{42°} 0.004 2 0.126 0.082	0.020 9 0.009 02 469 ^{50°} 339 0.035 7	0.018 4 0.0009 42 ^{70°} 406 ^{75°} 0.009 84 ^{73°}

4.8 SECTION 4

VAPOR PRESSURES

TABLE 4.2 Vapor Pressure of Mercury

Temp. °C	mm of Hg	Temp. °C	mm of Hg	Temp. °C	mm of Hg
0	0.000 185	78	0.078 89	158	3.873
		80	0.088 80	160	4.189
2	0.000 228				
4	0.000 276	82	0.1000		
6	0.000 335	84	0.1124	162	4.528
8	0.000 406	86	0.126 1	164	4.890
10	0.000 490	88	0.1413	166	5.277
		90	0.1582	168	5.689
12	0.000 588			170	6.128
14	0.000 706	92	0.1769		
16	0.000 846	94	0.1976	172	6.596
18	0.001 009	96	0.2202	174	7.095
20	0.001 201	98	0.2453	176	7.626
		100	0.2729	178	8.193
22	0.001 426			180	8.796
24	0.001 691	102	0.3032		
26	0.002 000	104	0.3366	182	9.436
28	0.002 359	106	0.3731	184	10.116
30	0.002 777	108	0.4132	186	10.839
		110	0.4572	188	11.607
32	0.003 261	112	0.5052	190	12.423
34	0.003 823	114	0.5576		
36	0.004 471	116	0.6150	192	13.287
38	0.005 219	118	0.6776	194	14.203
40	0.006 079	120	0.7457	196	15.173
				198	16.200
42	0.007 067	122	0.8198	200	17.287
44	0.008 200	124	0.9004		
46	0.009 497	126	0.9882		
48	0.010 98	128	1.084	202	18.437
50	0.012 67	130	1.186	204	19.652
				206	20.936
52	0.014 59	132	1.298	208	22.292
54	0.01677	134	1.419	210	23.723
56	0.019 25	136	1.551		
58	0.022 06	138	1.692	212	25.233
60	0.025 24	140	1.845	214	26.826
				216	28.504
62	0.028 83	142	2.010	218	30.271
64	0.032 87	144	2.188	220	32.133
66	0.037 40	146	2.379		
68	0.042 51	148	2.585		
70	0.048 25	150	2.807	222	34.092
				224	36.153
72	0.054 69	152	3.046	226	38.318
74	0.061 89	154	3.303	228	40.595
76	0.069 93	156	3.578	230	42.989

TABLE 4.2 Vapor Pressure of Mercury (continued)

Temp. °C	mm of Hg	Temp. °C	mm of Hg	Temp. °C	mm of Hg
232	45.503	302	257.78	372	994.34
234	48.141	304	269.17	374	1028.9
236	50.909	306	280.98	376	1064.4
238	53.812	308	293.21	378	1100.9
240	56.855	310	305.89	380	1138.4
242	60.044	312	319.02	382	1177.0
244	63.384	314	332.62	384	1216.6
246	66.882	316	346.70	386	1257.3
248	70.543	318	361.26	388	1299.1
250	74.375	320	376.33	390	1341.9
252	78.381	322	391.92	392	1386.1
254	82.568	324	408.04	394	1431.3
256	86.944	326	424.71	396	1477.7
258	91.518	328	441.94	398	1525.2
260	96.296	330	459.74	400	1574.1
262	101.28	332	478.13	430	2464
264	106.48	334	497.12	460	3715
266	111.91	336	516.74	490	5420
268	117.57	338	537.00		
270	123.47	340	557.90	520	7691
				550	10650
272	129.62	342	579.45	600	22.87 atm
274	136.02	344	601.69	650	35.49 atm
276	142.69	346	624.64	700	52.51 atm
278	149.64	348	648.30		
280	156.87	350	672.69	750	74.86 atm
				800	103.31 atm
282	164.39	352	697.83	850	138.42 atm
284	172.21	354	723.73	900*	180.92 atm
286	180.34	356	750.43	950	226.58 atm
288	188.79	358	777.92	1000	200.5
290	197.57	360	806.23	1000	290.5 atm
202	206.70	262	025.20	1050	358.1 atm
292 294	206.70 216.17	362 364	835.38 865.36	1100 1150	437.3 atm 521.3 atm
296 298	226.00 236.21	366 368	896.23 928.02	1200 1250	616.8 atm 721.4 atm
300	246.80	370	960.66	1300	835.9 atm
300	Z 1 0.00	370	200.00	1500	oss.7 auli

^{*}Critical point.

4.10 SECTION 4

TABLE 4.3 Vapor Pressure of Water for Temperatures from -10 to 120 °C

The values in the table are for water in contact with its own vapor. Where the water is in contact with air at a temperature t in degrees Celsius, the following correction must be added: Correction (when $t \le 40$ °C) = p(0.775 - 0.000313t)/100; correction (when t > 50 °C) = p(0.0652 - 0.0000875t)/100.

t, °C	p, mmHg						
-10.0	2.149	11.5	10.176	22.2	20.070	30.8	33.312
-9.5	2.236	12.0	10.518	22.4	20.316	31.0	33.695
-9.0	2.326	12.5	10.870	22.6	20.565	31.2	34.082
-8.5	2.418	13.0	11.231	22.8	20.815	31.4	34.471
-8.0	2.514	13.5	11.604	23.0	21.068	31.6	34.864
-7.5	2.613	14.0	11.987	23.2	21.324	31.8	35.261
-7.0	2.715	14.5	12.382	23.4	21.583	32.0	35.663
-6.5	2.822	15.0	12.788	23.6	21.845	32.2	36.068
-6.0	2.931	15.2	12.953	23.8	22.110	32.4	36.477
-5.5	3.046	15.4	13.121	24.0	22.387	32.6	36.891
-5.0	3.163	15.6	13.290	24.2	22.648	32.8	37.308
-4.5	3.284	15.8	13.461	24.4	22.922	33.0	37.729
-4.0	3.410	16.0	13.634	24.6	23.198	33.2	38.155
-3.5	3.540	16.2	13.809	24.8	23.476	33.4	38.584
-3.0	3.673	16.4	13.987	25.0	23.756	33.6	39.018
-2.5	3.813	16.6	14.166	25.2	24.039	33.8	39.457
-2.0	3.956	16.8	13.347	25.4	24.326	34.0	39.898
-1.5	4.105	17.0	14.530	25.6	24.617	34.2	40.344
-1.0	4.258	17.2	14.715	25.8	24.912	34.4	40.796
-0.5	4.416	17.4	14.903	26.0	25.209	34.6	41.251
0.0	4.579	17.6	15.092	26.2	25.509	34.8	41.710
0.5	4.750	17.8	15.284	26.4	25.812	35.0	42.175
1.0	4.926	18.0	15.477	26.6	26.117	35.2	42.644
1.5	5.107	18.2	15.673	26.8	26.426	35.4	43.117
2.0	5.294	18.4	15.871	27.0	26.739	35.6	43.595
2.5	5.486	18.6	16.071	27.2	27.055	35.8	44.078
3.0	5.685	18.8	16.272	27.4	27.374	36.0	44.563
3.5	5.889	19.0	16.477	27.6	27.696	36.2	45.054
4.0	6.101	19.2	16.685	27.8	28.021	36.4	45.549
4.5	6.318	19.4	16.894	28.0	28.349	36.6	46.050
5.0	6.543	19.6	17.105	28.2	28.680	36.8	46.556
5.5	6.775	19.8	17.319	28.4	29.015	37.0	47.067
6.0	7.013	20.0	17.535	28.6	29.354	37.2	47.582
6.5	7.259	20.2	17.753	28.8	29.697	37.4	48.102
7.0	7.513	20.4	17.974	29.0	30.043	37.6	48.627
7.5	7.775	20.6	18.197	29.2	30.392	37.8	49.157
8.0	8.045	20.8	18.422	29.4	30.745	38.0	49.692
8.5	8.323	21.0	18.650	29.6	31.102	38.2	50.231
9.0	8.609	21.2	18.880	29.8	31.461	38.4	50.774
9.5	8.905	21.4	19.113	30.0	31.824	38.6	51.323
10.0	9.209	21.6	19.349	30.2	32.191	38.8	51.879
10.5	9.521	21.8	19.587	30.4	32.561	39.0	52.442
11.0	9.844	22.0	19.827	30.6	32.934	39.2	53.009

TABLE 4.3 Vapor Pressure of Water for Temperatures from -10 to 120 °C (continued)

t, °C	p, mmHg						
39.4	54.580	58.5	139.34	78.5	334.2	96.4	667.31
39.6	54.156	59.0	142.60	79.0	341.0	96.6	672.20
39.8	54.737	59.5	145.99	79.5	348.1	96.8	677.12
40.0	55.324	60.0	149.38	80.0	355.1	970	682.07
40.5	56.81	60 5	152.91	80.5	362.4	97.2	687.04
41.0	58 34	61.0	156.43	81.0	369.7	97.4	692.05
41.5	59.90	61.5	160.10	81.5	377.3	97.6	697.10
42.0	61.50	62.0	163.27	82.0	384.9	97.8	702.17
42.5	63.13	62.5	167.58	82.5	392.8	98.0	707.27
43.0	64.80	63.0	171.38	83.0	400.6	98.2	712.40
43.5	66.51	63.5	175.35	83.5	408.7	98.4	717.56
44.0	68.26	64.0	179.31	84.0	416.8	98.6	722.75
44.5	70.05	64.5	183.43	84.5	425.2	98.8	727.98
45.0	71.88	65.0	187.54	85.0	433.6	99.0	733.24
45.5	73.74	65.5	191.82	85.5	442.3	99.2	738.53
46.0	75.65	66.0	196.09	86.0	450.9	99.4	743.85
46.5	77.61	66.5	200.53	86.5	459.8	99.6	749.20
47.0	79.60	67.0	204.96	87.0	468.7	99.8	754.58
47.5	81.64	67.5	209.57	87.5	477.9	100.0	760.00
48.0	83.71	68.0	214.17	88.0	487.1	101.0	787.57
48.5	85.85	68.5	218.95	88.5	496.6	102.0	815.86
49.0	88.02	69.0	223.73	89.0	506.1	103.0	845.12
49.5	90.24	69.5	228.72	89.5	515.9	104.0	875.06
50.0	92.51	70.0	233.7	90.0	525.76	105.0	906.07
50.5	94.86	70.5	238.8	90.5	535.83	106.0	937.92
51.0	97.20	71.0	243.9	91.0	546.05	107.0	970.60
51.5	99.65	71.5	249.3	91.5	556.44	108.0	1004.42
52.0	102.09	72.0	254.6	92.0	566.99	109.0	1038.92
52.5	104.65	72.5	260.2	92.5	577.71	110.0	1074.56
53.0	107.20	73.0	265.7	93.0	588.60	111.0	1111.20
53.5	109.86	73.5	271.5	93.5	599.66	112.0	1148.74
54.0	112.51	74.0	277.2	94.0	610.90	1130	1187.42
54.5	115.28	74.5	283.2	94.5	622.31	114.0	1227.25
55.0	118.04	75.0	289.1	95.0	633.90	115.0	1267.98
55.5	120.92	75.5	295.3	95.2	638.59	116.0	1309.94
56.0	123.80	76.0	301.4	95.4	643.30	117.0	1352.95
56.5	126.81	76.5	307.7	95.6	648.05	118.0	1397.18
57.0	129.82	77.0	314.1	95.8	652.82	119.0	1442.63
57.5	132.95	77.5	320.7	96.0	657.62	120.0	1489.14
58.0	136.08	78.0	327.3	96.2	662.45		

4.12 SECTION 4

 TABLE 4.4
 Vapor Pressure of Deuterium Oxide

t, °C	p, mmHg	t, °C	p, mmHg	t, °C	p, mmHg
0 1 2 3 3.8 10	3.65 3.93 4.29 4.65 5.05 7.79	20 30 40 50 60 70	15.2 28.0 49.3 83.6 136.6 216.1	80 90 100 101.43	331.6 495.5 722.2 760.0

BOILING POINTS

 TABLE 4.5A
 Boiling Points for Common Organic Solvents

Arranged in order of increasing boiling point

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Ethylene oxide	10.6	Oxirane	Benzene	80.1	
Chloroethane	12.3	Ethyl chloride	Cyclohexane	80.7	
Furan	31.4		Propyl formate	80.9	
Methyl formate	31.5		Acetonitrile	81.6	
Diethyl ether	34.6	Ethyl ether	2-Propanol	82.4	Isopropyl alcohol
Propylene oxide	34.5		1,1-Dimethylethanol	82.4	t-Butanol
Pentane	36.1		Cyclohexene	83.0	
Bromoethane	38.4	Ethyl bromide	Diisopropyl amine	83.5	
Dichloromethane	39.8	Methylene chloride	1,2-Dichloroethane	83.7	
Dimethoxyethane	42.3	DME, glyme	Thiophene	84.2	
Carbon disulfide	46.3		Trichloroethylene	87.2	
1-Isopropoxy-	47.9		Isopropyl acetate	88.2	
2-propanol			1-Bromo-	91.5	Isobutyl bromide
Ethyl formate	54.2		2-methylpropane		
Acetone	56.2	Dimethyl ketone	2,5-Dimethylfuran	93-94	
Methyl acetate	56.3		Ethyl chloroformate	94.0	
1,1-Dichloroethane	57.3		Allyl alcohol	96.6	
Dichloroethylene	60.6		1,2-Dichloropropane	96.8	
Chloroform	61.2		1-Propanol	97.2	n-Propyl alcohol
Methanol	64.7		Heptane	98.4	
Tetrahydrofuran	66.0	THF	1-Chloro-		
Diisopropyl ether	68.0	Isopropyl ether	3-methylbutane	99.0	
Hexane	68.7		Ethyl propanoate	99.1	Ethyl propionate
1-Chloro-	68.9	Isobutyl chloride	2-Butanol	99.6	sec-Butanol
2-methylpropane			Formic acid	100.8	
1,1,1-Trichloroethane	74.0		Methylcyclohexane	100.9	
1,3-Dioxolane	74-75		1,4-Dioxane	101.2	
Carbon tetrachloride	76.7		Nitromethane	101.2	
Ethyl acetate	77.1		Propyl acetate	101.5	
1-Chlorobutane	77.9	Butyl chloride	2-Pentanone	101.7	Methyl propyl
Ethanol	78.3	•			ketone
2-Butanone	79.6	Methyl ethyl ketone	3-Pentanone	102.0	Diethyl ketone
2-Methyltetrahy-	80.0		2-Methyl-2-butanol	102.0	t-Pentanol
drofuran			1,1-Diethoxyethane	102.7	

TABLE 4.5A Boiling Points for Common Organic Solvents (continued)

Arranged in order of increasing boiling point

Compound name	bp (°C)	Other name	Compound name b	p (°C)	Other name
Butyl formate	106.6		4-Heptanone	143.7	Dipropyl ketone
2-Methyl-1-propanol	107.9	Isobutanol	o-Xylene	144.4	1,2-
Toluene	110.6	Methylbenzene			Dimethylbenzene
sec-Butyl acetate	112.3		2-Methoxyethyl	144.5	
1,1,2-Trichloroethane	113.5		acetate		
Nitroethane	114.1		1,1,2, 2-		
Pyridine	115.2		Tetrachloroethane	146.3	
3-Pentanol	115.6		3-Heptanone	147.8	Ethyl butyl ketone
4-Methyl-2-pentanone	115.7	Methyl isobutyl	Tribromomethane	149.6	Bromoform
		ketone	Nonane	150.8	
1-Chloro-2, 3-epoxypropane	116.1	Epichlorohydrin	2-Heptanone	151	Methyl pentyl ketone
1-Butanol	117.7		Isopropylbenzene	152.4	Cumene
Acetic acid	117.9		N,N-Dimethyl-		
Isobutyl acetate	118.0		formamide	153.0	DMF
2-Pentanol	119.3	sec-Pentanol	Methoxybenzene	153.8	Anisole
1-Bromo-			Ethyl lactate	154.5	
3-methylbutane	119.7	Isopentyl bromide	Cyclohexanone	155.7	
1-Methoxy-2-propano			Bromobenzene	156.2	
2-Nitropropane		Nitroisopropane	1,2,3-	156.9	
Tetrachloroethylene	121.1		Trichloropropane		
Ethyl butanoate	121.6	Ethyl butyrate	1-Hexanol	157.5	
3-Hexanone	123	Ethyl propyl ketone	Propylbenzene	159.2	
2,4-Dimethyl-	124	Diisopropyl ketone	Cyclohexanol	161.1	
3-pentanone			Bis(2-methoxyethyl)	160	Diglyme
2-Methoxyethanol	124.6		ether		8-7
Octane	125.7		Isopentyl propanoate	160.2	Isopentyl
Butyl acetate	126.1				propionate
Diethyl carbonate	126.8		2-Heptanol	160.4	rr
2-Hexanone		Methyl butyl ketone	Pentachloroethane	160.5	
1-Chloro-2-propanol	127.4		2-Furaldehyde		Furfural
2-Chloroethanol	128.6		2,6-Dimethyl-		
1-Nitropropane	131.2		4-heptanone	168.1	Diisobutyl
Chlorobenzene	131.7				ketone
1,2-Dibromoethane	131.7		4-Hydroxy-4-methyl-	169.2	
4-Methyl-2-pentanol	131.7		2-pentanone		
3-Methyl-1-butanol	132.0		2-Furanmethanol	170.0	2-Hydroxy
Cyclohexylamine		Aminocyclohexane			methylfuran
2-Ethoxyethanol	134.8		Ethoxybenzene	170	Phenetole
Ethylbenzene	136.2		2-Butoxyethanol		Butyl cellosolve
1-Pentanol	138		Diisopentyl ether	173.4	Butyreeneserve
p-Xylene	138.4	1.4-	Decane	174.2	
r j		Dimethylbenzene	1,3-Dichloro-	174.3	
m-Xylene	139.1	•	2-propanol	17 110	
m Hylene	137.1	Dimethylbenzene	Cyclohexyl acetate	174–1	75
Acetic anhydride	140.0	2 micai, tootheire	1-Heptanol	175.8	
2,4-Pentanedione		Acetylacetone	Furfuryl acetate	175-1	77
Isopentyl acetate	142	1 icety factions	4-Isopropyl-	177.1	<i>p</i> -Cymene
Dibutyl ether	142.4		1-methylbenzene	1,7.1	Political
Dioutyl Cilici	172.4		1-memy rochizene		

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TABLE 4.5A Boiling Points for Common Organic Solvents (*continued*)

Arranged in order of increasing boiling point

Compound name	bp (°C) Other name	Compound name	bp (°C)	Other name
Isopentyl butanoate		Isopentyl butyrate	o-Chloroaniline	208.8	1-Amino-
Bis(2-chloroethyl)	178.8	Dichloro diethyl			2-chlorobenzene
ether		ether	Nitrobenzene	210.8	
2-Octanol	179		Ethyl benzoate	212.4	
1,2-Dichlorobenzene	180.4	o-Dichlorobenzene	Isophorone	215.2	3,5, 5-
Ethyl acetoacetate	180.8				Trimethylcyclo-
Phenol	181.8	Hydroxybenzene			hex-2-en-1-one
2-Ethyl-1-hexanol	184.3		Naphthalene	217.7	
Aniline	184.4	Aminobenzene	2-(2-Ethoxyethoxy)	218.5	
Benzyl ethyl ether	185.0		ethyl acetate		
Diethyl oxalate	185.4		Acetamide	221.2	
1,2-Propanediol	188	Propylene glycol	Methyl salicylate	223.0	
Bis(2-ethoxyethyl)	188.4	1, 0,	Diethyl maleate	225.3	
ether			1,4-Butanediol	230	
Dimethylsulfoxide	189.0	DMSO	Propyl benzoate	231.2	
1,2-Ethanediol	190.2	Diacetoxyethane	1-Decanol	230.2	
diacetate		,	Phenylacetonitrile		Cyano-
Benzonitrile	191.0	Cyanobenzene			methylbenzene
2,5-Hexanedione	191.4	-,	Quinoline	237	,
2-(2-Methoxyethoxy)			Tributyl borate	238.5	
ethanol	1,		Propylene carbonate	240	
<i>N</i> , <i>N</i> -Dimethylaniline	194.2	Dimethyl-	2-Phenoxyethanol	240	
11,11 Dimentylamine	171.2	aminobenzene	Bis(2-hydroxyethyl)	245	Diethylene glycol
1-Octanol	195.2	ammoochzene	ether	243	Dietifylene grycor
1,2-Ethanediol		Ethylene glycol	Dibutyl oxalate	245.5	
Diethyl malonate	199.3	Euryrene grycor	Butyl benzoate	250	
Methyl benzoate	199.5		1,2,3-Propanetriol		Glycerol
o-Toluidine		1-Amino-	triacetate	259	triacetate
0-Totuldilic	200.4	2-methylbenzene	1-Chloronaphthalene	259.3	triacctate
<i>p</i> -Toluidine	200.6	1-Amino-	Isopentyl benzoate	262	
p-Torundine	200.0	4-methylbenzene	trans-Ethyl cinnamate		
2-(2-Ethoxyethoxy)	202	4-memyroenzene	Bis (2-(2-methoxy-		Tui alama
ethanol	202		ethoxy)-	213.3	Triglyme
	202.1	Mathed who wil	• • • • • • • • • • • • • • • • • • • •		
Acetophenone	202.1	Methyl phenyl- ketone	ethyl) ether	277	
1.2 Dil	202.6	ketone	1-Methoxy-	277	
1,2-Dibutoxyethane	203.6	Dl (1. 1 . 1 1 1	2-nitrobenzene	277	
1,2-Phenylethanol		Phenethyl alcohol	Isopentyl salicylate	277-	
<i>m</i> -Toluidine	203.4	1-Amino-		278	
	205.5	3-methylbenzene	1-Bromonaphthalene	281.1	100:4
Benzyl alcohol	205.5	Hydroxy-	Dimethyl o -phthalate	283.7	1,2-Bis(carbo-
		methylbenzene			methoxy)
Camphor	207	1,7,7-Trimethyl-			benzene
		bicyclo[2.2.1]	2,2'-(Ethylenedioxy)		
		heptan-2-one	bisethanol	285	
1,3-Butanediol	207.5		Glycerol	290	
1,2,3,4-Tetrahy-	207.6	Tetralin	Diethyl o-phthalate	295	
dronaphthalene			Benzyl benzoate	323.5	
γ -Valerolactone	207-		Dibutyl o-phthalate	340.0	
	208		Dibutyl decanedioate	344-34	45

 TABLE 4.5B
 Boiling Points for Common Organic Solvents

Arranged alphabetically by solvent name

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Acetamide	221.2		Chlorobenzene	131.7	
Acetic acid	117.9		1-Chlorobutane	77.9	Butyl chloride
Acetic anhydride	140.0		1-Chloro-2,	116.1	Epichlorohydrin
Acetone	56.2	Dimethyl ketone	3-epoxypropane		
Acetonitrile	81.6		1-Chloro-2-propanol	127.4	
Acetophenone	202.1	Methyl phenyl	Chloroethane	12.3	Ethyl chloride
_		ketone	2-Chloroethanol	128.6	
Allyl alcohol	96.6		Chloroform	61.2	
Aniline	184.4	Aminobenzene	1-Chloro-		
Benzene	80.1		3-methylbutane	99.0	
Benzonitrile	191.0	Cyanobenzene	1-Chloro-	68.9	Isobutyl chloride
Benzyl alcohol	205.5	Hydroxy-	2-methylpropane		
		methylbenzene	1-Chloronaphthalene	259.3	
Benzyl benzoate	323.5		Cyclohexane	80.7	
Benzyl ethyl ether	185.0		Cyclohexanol	161.1	
Bis(2-(2-methoxy-	275.3	Triglyme	Cyclohexanone	155.7	
ethoxy)-			Cyclohexene	83.0	
ethyl) ether			Cyclohexyl acetate	174-	
Bis(2-chloroethyl)	178.8	Dichloro		175	
ether		diethyl ether	Cyclohexylamine	134.8	Aminocyclohexane
Bis(2-ethoxyethyl)	188.4		Decane	174.2	
ether			1-Decanol	230.2	
Bis(2-hydroxyethyl)	245	Diethylene glycol	1,2-Dibromoethane	131.7	
ether			1,2-Dibutoxyethane	203.6	
Bis(2-methoxyethyl) ether	160	Diglyme	Dibutyl decanedioate	344– 345	
Bromobenzene	156.2		Dibutyl ether	142.4	
Bromoethane	38.4	Ethyl bromide	Dibutyl o-phthalate	340.0	
1-Bromo-	91.5	Isobutyl bromide	Dibutyl oxalate	245.5	
2-methylpropane	71.0	1500aty1010111ac	1,2-Dichlorobenzene		o-Dichlorobenzene
1-Bromo-	119.7	Isopentyl bromide	Dichloroethylene	60.6	
3-methylbutane			Dichloromethane	39.8	Methylene chloride
1-Bromonaphthalene	281.1		1,1-Dichloroethane	57.3	
1,3-Butanediol	207.5		1,2-Dichloroethane	83.7	
1,4-Butanediol	230		1,2-Dichloropropane	96.8	
1-Butanol	117.7		1,3-Dichloro-	174.3	
2-Butanol	99.6	sec-Butanol	2-propanol		
2-Butanone	79.6	Methyl ethyl ketone	1,1-Diethoxyethane	102.7	
2-Butoxyethanol	170.2	Butyl cellosolve	Diethyl carbonate	126.8	
Butyl acetate	126.1		Diethyl ether	34.6	Ethyl ether
sec-Butyl acetate	112.3		Diethyl maleate	225.3	
Butyl benzoate	250		Diethyl malonate	199.3	
Butyl formate	106.6		Diethyl o-phthalate	295	
Camphor	207	1,7,7-Trimethylbi-	Diethyl oxalate	185.4	
=		cyclo [2.2.1]	Diisopentyl ether	173.4	
		heptan-2-one	Diisopropyl amine	83.5	
Carbon disulfide	46.3		Diisopropyl ether	68.0	Isopropyl ether
Carbon tetrachloride	76.7		Dimethoxyethane	42.3	DME, glyme
o-Chloroaniline	208.8	1-Amino-			
		2-chlorobenzene			

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TABLE 4.5B Boiling Points for Common Organic Solvents (continued)

Arranged alphabetically by solvent name

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
<i>N,N</i> -Dimethylaniline	194.2	Dimethyl- aminobenzene	2-Heptanone	151	Methyl pentyl ketone
1,1-Dimethylethanol	82.4	t-Butanol	3-Heptanone	147.8	Ethyl butyl ketone
N,N-Dimethyl-	153.0	DMF	4-Heptanone	143.7	Dipropyl ketone
formamide			Hexane	68.7	
2,5-Dimethylfuran	93-94		2,5-Hexanedione	191.4	
2,6-Dimethyl-			1-Hexanol	157.5	
4-heptanone	168.1	Diisobutyl ketone	2-Hexanone	127.2	Methyl butyl ketone
2,4-Dimethyl-			3-Hexanone	123	Ethyl propyl ketone
3-pentanone	124	Diisopropyl ketone	4-Hydroxy-4-methyl-		
Dimethyl o-phthalate	283.7	1,2-Bis(carbo-	2-pentanone	169.2	
		methoxy)benzene	Isobutyl acetate	118.0	
Dimethylsulfoxide	189.0	DMSO	Isopentyl acetate	142	
1,4-Dioxane	101.2		Isopentyl benzoate	262	
1,3-Dioxolane	74–75		Isopentyl butanoate	178.6	Isopentyl butyrate
1,2-Ethanediol	197.3	Ethylene glycol	Isopentyl propanoate	160.2	Isopentyl
1,2-Ethanediol	190.2	Diacetoxyethane			propionate
diacetate			Isopentyl salicylate	277-	
Ethoxybenzene	170	Phenetole		278	
2-Ethoxyethanol	134.8		Isophorone	215.2	3,5,5-Trimethylcycl-
2-(2-Ethoxyethoxy)	202				ohex-2-en-1-one
ethanol			Isopropyl acetate	88.2	
2-(2-Ethoxyethoxy)	218.5		Isopropylbenzene		Cumene
ethyl acetate			1-Isopropoxy-	47.9	
Ethyl acetate	77.1		2-propanol		
Ethyl acetoacetate	180.8		4-Isopropyl-	177.1	p -Cymene
Ethyl benzoate	212.4		1-methylbenzene		
Ethyl butanoate		Ethyl butyrate	Methanol	64.7	
Ethyl chloroformate	94.0		Methoxybenzene		Anisole
trans-Ethyl cinnamate			Methyl acetate	56.3	
Ethyl formate	54.2		Methyl benzoate	199.5	
Ethyl lactate	154.5		Methyl formate	31.5	
Ethyl propanoate	99.1	Ethyl propionate	Methyl salicylate	223.0	
Ethylbenzene	136.2	0.1	Methylcyclohexane	100.9	
Ethylene oxide	10.6	Oxirane	1-Methoxy-	277	
2,2'-(Ethylenedioxy)	205		2-nitrobenzene	1 120 1	
bisethanol	285		1-Methoxy-2-propand		
2-Ethyl-1-hexanol	184.3 100.8		2-(2-Methoxyethoxy)	194.1	
Formic acid		Frankram 1	ethanol	1246	
2-Furaldehyde Furan	31.4	Furfural	2-Methoxyethanol 2-Methoxyethyl aceta	124.6	
2-Furanmethanol		2-Hydroxy-	2-Methyl-1-propanol		Isobutanol
2-1 uranineuranor	170.0	methylfuran	2-Methyl-2-butanol		t-Pentanol
Furfuryl acetate	175-	memynuran	2-Methyltetrahy-	80.0	t-r cittatioi
r urrur yr acctate	173		drofuran	00.0	
Glycerol	290		3-Methyl-1-butanol	132.0	
Heptane	98.4		4-Methyl-2-pentanol	131.7	
1-Heptanol	175.8		4-Methyl-2-pentanon		Methyl isobutyl
2-Heptanol	160.4		pentanon	- 110.7	ketone
10p.m	100.7				

TABLE 4.5B Boiling Points for Common Organic Solvents (*continued*)

Arranged alphabetically by solvent name

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Naphthalene	217.7		Propyl formate	80.9	
Nitrobenzene	210.8		Propylbenzene	159.2	
Nitroethane	114.1		Pyridine	115.2	
Nitromethane	101.2		Quinoline	237	
1-Nitropropane	131.2		1,1,2,2-Tetra-	146.3	
2-Nitropropane	120.3	Nitroisopropane	chloroethane		
Nonane	150.8		Tetrachloroethylene	121.1	
Octane	125.7		Tetrahydrofuran	66.0	THF
1-Octanol	195.2		Thiophene	84.2	
2-Octanol	179		Toluene	110.6	Methylbenzene
Pentachloroethane	160.5		o-Toluidine	200.4	1-Amino-
Pentane	36.1				2-methylbenzene
2,4-Pentanedione	140.6	Acetylacetone	m-Toluidine	203.4	1-Amino-
1-Pentanol	138				3-methylbenzene
2-Pentanol	119.3	sec-Pentanol	p-Toluidine	200.6	1-Amino-
3-Pentanol	115.6				4-methylbenzene
2-Pentanone	101.7	Methyl propyl	Tribromomethane	149.6	Bromoform
		ketone	Tributyl borate	238.5	
3-Pentanone	102.0	Diethyl ketone	1,1,1-Trichloroethane	74.0	
Phenol	181.8	Hydroxybenzene	1,1,2-Trichloroethane	113.5	
2-Phenoxyethanol	240		Trichloroethylene	87.2	
Phenylacetonitrile	233.5	Cyano-	1,2,3,4-Tetrahy-	207.6	Tetralin
		methylbenzene	dronaphthalene		
1-Phenylethanol	203.9	Phenethyl alcohol	1,2,3-Trichloro	156.9	
1,2-Propanediol	188	Propylene glycol	propane		
1,2,3-Propanetriol	258-	Glycerol	γ-Valerolactone	207-	
triacetate	259	triacetate		208	
1-Propanol	97.2	n-Propyl alcohol	o-Xylene	144.4	1,2-Dimethyl-
2-Propanol	82.4	Isopropyl alcohol			benzene
Propylene carbonate	240		m-Xylene	139.1	1,3-Dimethyl-
Propylene oxide	34.5				benzene
Propyl acetate	101.5		p-Xylene	138.4	1,4-Dimethyl-
Propyl benzoate	231.2				benzene

TABLE 4.5C Boiling Points for Common Organic Solvents Arranged by compound type in order of increasing boiling point

	Compound name	(°C)	Other name
acid	Formic acid	100.8	
acid	Acetic acid	117.9	
alcohol	1-Isopropoxy-2-propanol	47.9	
alcohol	Methanol	64.7	
alcohol	Ethanol	78.3	
alcohol	2-Propanol	82.4	Isopropyl alcohol
alcohol	1,1-Dimethylethanol	82.4	t-Butanol
alcohol	Allyl alcohol	96.6	

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TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)

	Compound name	(°C)	Other name
alcohol	1-Propanol	97.2	n-Propyl alcohol
alcohol	2-Butanol	99.6	sec-Butanol
alcohol	2-Methyl-2-butanol	102.0	t-Pentanol
alcohol	2-Methyl-1-propanol	107.9	Isobutanol
alcohol	3-Pentanol	115.6	
alcohol	1-Butanol	117.7	
alcohol	2-Pentanol	119.3	sec-Pentanol
alcohol	1-Methoxy-2-propanol	120.1	
alcohol	2-Methoxyethanol	124.6	
alcohol	1-Chloro-2-propanol	127.4	
alcohol	2-Chloroethanol	128.6	
alcohol	4-Methyl-2-pentanol	131.7	
alcohol	3-Methyl-1-butanol	132.0	
alcohol	2-Ethoxyethanol	134.8	
alcohol	1-Pentanol	138	
alcohol	1-Hexanol	157.5	
alcohol	Cyclohexanol	161.1	
alcohol	2-Heptanol	160.4	
alcohol	4-Hydroxy-4-methyl-2-pentanone	169.2	
alcohol	2-Furanmethanol	170.0	2-Hydroxymethylfuran
alcohol	2-Butoxyethanol	170.2	Butyl cellosolve
alcohol	1,3-Dichloro-2-propanol	174.3	Butyleenosolve
alcohol	1-Heptanol	175.8	
alcohol	2-Octanol	179	
alcohol	Phenol	181.8	Hydroxybenzene
alcohol	2-Ethyl-1-hexanol	184.3	Trydroxybenizene
alcohol	1,2-Propanediol	188	Propylene glycol
alcohol	2-(2-Methoxyethoxy) ethanol	194.1	r ropylene grycor
alcohol	1-Octanol	195.2	
alcohol	1,2-Ethanediol	193.2	Ethylene glycol
alcohol		202	Emylene grycor
alcohol	2-(2-Ethoxyethoxy) ethanol		Dhanathad alaah al
alcohol	1-Phenylethanol Benzyl alcohol	203.9 205.5	Phenethyl alcohol Hydroxymethylbenzene
	•		Hydroxymethylbelizene
alcohol alcohol	1,3-Butanediol	207.5 223.0	
	Methyl salicylate		
alcohol	1,4-Butanediol	230	
alcohol	1-Decanol	230.2	
alcohol	2-Phenoxyethanol	240	D: 4.1 1 1
alcohol	Bis(2-hydroxyethyl) ether	245	Diethylene glycol
alcohol	Isopentyl salicylate	277–278	
alcohol	2,2'-(Ethylenedioxy)bisethanol	285	
alcohol	Glycerol	290	T 6 1
aldehyde	2-Furaldehyde	161.8	Furfural
amide	<i>N,N</i> -Dimethylformamide	153.0	DMF
amide	Acetamide	221.2	
amine	Diisopropylamine	83.5	
amine	Pyridine	115.2	

 $\textbf{TABLE 4.5C} \quad \text{Boiling Points for Common Organic Solvents } (continued)$

	Compound name	(°C)	Other name
amine	Cyclohexylamine	134.8	Aminocyclohexane
amine	Aniline	184.4	Aminobenzene
amine	N,N-Dimethylaniline	194.2	Dimethylaminobenzene
amine	o-Toluidine	200.4	1-Amino- 2-methylbenzene
amine	<i>p</i> -Toluidine	200.6	1-Amino- 4-methylbenzene
amine	<i>m</i> -Toluidine	203.4	1-Amino-
amine	o-Chloroaniline	208.8	3-methylbenzene 1-Amino-2-chlorobenzene
amine	Ouinoline Ouinoline	237	1-Ammo-2-emorobenzene
anhydride	Acetic anhydride	140.0	
bromide	Bromoethane	38.4	Ethyl bromida
bromide		91.5	Ethyl bromide
	1-Bromo-2-methylpropane		Isobutyl bromide
bromide	1-Bromo-3-methylbutane	119.7	Isopentyl bromide
bromide	1,2-Dibromoethane	131.7	D
bromide	Tribromomethane	149.6	Bromoform
bromide	Bromobenzene	156.2	
bromide	1-Bromonaphthalene	281.1	ma 1 11 11
chloride	Chloroethane	12.3	Ethyl chloride
chloride	Dichloromethane	39.8	Methylene chloride
chloride	1,1-Dichloroethane	57.3	
chloride	Dichloroethylene	60.6	
chloride	Chloroform	61.2	
chloride	1-Chloro-2-methylpropane	68.9	Isobutyl chloride
chloride	1,1,1-Trichloroethane	74.0	
chloride	Carbon tetrachloride	76.7	
chloride	1-Chlorobutane	77.9	Butyl chloride
chloride	1,2-Dichloroethane	83.7	
chloride	Trichloroethylene	87.2	
chloride	1,2-Dichloropropane	96.8	
chloride	1-Chloro-3-methylbutane	99.0	
chloride	1,1,2-Trichloroethane	113.5	
chloride	1-Chloro-2,3-epoxypropane	116.1	Epichlorohydrin
chloride	Tetrachloroethylene	121.1	
chloride	1-Chloro-2-propanol	127.4	
chloride	2-Chloroethanol	128.6	
chloride	Chlorobenzene	131.7	
chloride	1,1,2,2-Tetrachloroethane	146.3	
chloride	1,2,3-Trichloropropane	156.9	
chloride	Pentachloroethane	160.5	
chloride	1,3-Dichloro-2-propanol	174.3	
chloride	Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether
chloride	1,2-Dichlorobenzene	180.4	o-Dichlorobenzene
chloride	o-Chloroaniline	208.8	1-Amino-2-chlorobenzene
chloride	1-Chloronaphthalene	259.3	
ester	Methyl formate	31.5	
ester	Ethyl formate	54.2	

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TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)

	Compound name	(°C)	Other name
ester	Methyl acetate	56.3	
ester	Ethyl acetate	77.1	
ester	Propyl formate	80.9	
ester	Isopropyl acetate	88.2	
ester	Methyl chloroformate	94.0	
ester	Ethyl propanoate	99.1	Ethyl propionate
ester	Propyl acetate	101.5	
ester	Butyl formate	106.6	
ester	sec-Butyl acetate	112.3	
ester	Isobutyl acetate	118.0	
ester	Ethyl butanoate	121.6	Ethyl butyrate
ester	Butyl acetate	126.1	3
ester	Diethyl carbonate	126.8	
ester	Isopentyl acetate	142	
ester	2-Methoxyethyl acetate	144.5	
ester	Ethyl lactate	154.5	
ester	Isopentyl propanoate	160.2	Isopentyl propionate
ester	Cyclohexyl acetate	174–175	
ester	Furfuryl acetate	175–177	
ester	Isopentyl butanoate	178.6	Isopentyl butyrate
ester	Ethyl acetoacetate	180.8	
ester	Diethyl oxalate	185.4	
ester	1.2-Ethanediol diacetate	190.2	Diacetoxyethane
ester	Diethyl malonate	199.3	
ester	Methyl benzoate	199.5	
ster	γ-Valerolactone	207–208	
ester	Ethyl benzoate	212.4	
ester	2-(2-Ethoxyethoxy)ethyl acetate	218.5	
ester	Methyl salicylate	223.0	
ester	Diethyl maleate	225.3	
ester	Propyl benzoate	231.2	
ester	Propylene carbonate	240	
ester	Dibutyl oxalate	245.5	
ester	Butyl benzoate	250	
ester	1,2,3-Propanetriol triacetate	258–259	Glycerol triacetate
ester	Isopentyl benzoate	262	Gryceror triacetate
ester	trans-Ethyl cinnamate	271.0	
ester	Isopentyl salicylate	277–278	
ester	Dimethyl o -phthalate	283.7	1,2-Bis(carbomethoxy)
	• •		benzene
ester	Diethyl o -phthalate	295	
ester	Benzyl benzoate	323.5	
ester	Dibutyl o-phthalate	340.0	
ester	Dibutyl decanedioate	344–345	
ether	Ethylene oxide	10.6	Oxirane
ether	Furan	31.4	

 $\textbf{TABLE 4.5C} \quad \text{Boiling Points for Common Organic Solvents} \, (continued)$

	Compound name	(°C)	Other name
ether	Diethyl ether	34.6	Ethyl ether
ether	Propylene oxide	34.5	
ether	Dimethoxyethane	42.3	DME, glyme
ether	1-Isopropoxy-2-propanol	47.9	
ether	Tetrahydrofuran	66.0	THF
ether	Diisopropyl ether	68.0	Isopropyl ether
ether	1,3-Dioxolane	74–75	
ether	2-Methyltetrahydrofuran	80.0	
ether	2,5-Dimethylfuran	93-94	
ether	1,4-Dioxane	101.2	
ether	1,1-Diethoxyethane	102.7	
ether	1-Chloro-2,3-epoxypropane	116.1	Epichlorohydrin
ether	1-Methoxy-2-propanol	120.1	
ether	2-Methoxyethanol	124.6	
ether	2-Ethoxyethanol	134.8	
ether	Dibutyl ether	142.4	
ether	2-Methoxyethyl acetate	144.5	
ether	Methoxybenzene	153.8	Anisole
ether	Bis(2-methoxyethyl) ether	160	Diglyme
ether	2-Furanmethanol	170.0	2-Hydroxymethylfuran
ether	Ethoxybenzene	170	Phenetole
ether	2-Buroxyethanol	170.2	Butyl cellosolve
ether	Diisopentyl ether	173.4	,
ether	Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether
ether	Benzyl ethyl ether	185.0	•
ether	Bis(2-ethoxyethyl)ether	188.4	
ether	2-(2Methoxyethoxy)ethanol	194.1	
ether	2-(2-Ethoxyethoxy) ethanol	202	
ether	1,2 Dibutoxyethane	203.6	
ether	2-(2-Ethoxyethoxy)ethyl acetate	218.5	
ether	2-Phenoxyethanol	240	
ether	Bis(2-hydroxyethyl) ether	245	Diethylene glycol
ether	Bis(2-(2-methoxyethoxy)-	275.3	Triglyme
	ethyl) ether		8,7
ether	1-Methoxy-2-nitrobenzene	277	
ether	2,2'-(Ethylenedioxy) bisethanol	285	
hydrocarbon	Pentane	36.1	
hydrocarbon	Hexane	68.7	
hydrocarbon	Benzene	80.1	
hydrocarbon	Cyclohexane	80.7	
hydrocarbon	Cyclohexene	83.0	
hydrocarbon	Heptane	98.4	
hydrocarbon	Methylcyclohexane	100.9	
hydrocarbon	Toluene	110.6	Methylbenzene
hydrocarbon	Octane	125.7	inedity to enizetic
hydrocarbon	Ethylbenzene	136.2	
nydrocarbon	p -Xylene	138.4	1,4-Dimethylbenzene

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 TABLE 4.5C
 Boiling Points for Common Organic Solvents (continued)

	Compound name	(°C)	Other name
hydrocarbon	o-Xylene	144.4	1,2-Dimethylbenzene
hydrocarbon	Nonane	150.8	
hydrocarbon	Isopropylbenzene	152.4	Cumene
hydrocarbon	Propylbenzene	159.2	
hydrocarbon	Decane	174.2	
hydrocarbon	4-Isopropyl-1-methylbenzene	177.1	<i>p</i> -Cymene
hydrocarbon	1,2,3,4-Tetrahydronaphthalene	207.6	Tetralin
hydrocarbon	Naphthalene	217.7	
ketone	Acetone	56.2	Dimethyl ketone
ketone	2-Butanone	79.6	Methyl ethyl ketone
ketone	2-Pentanone	101.7	Methyl propyl ketone
ketone	3-Pentanone	102.0	Diethyl ketone
ketone	4-Methyl-2-pentanone	115.7	Methyl isobutyl ketone
ketone	3-Hexanone	123	Ethyl propyl ketone
ketone	2,4-Dimethyl-3-pentanone	124	Diisopropyl ketone
ketone	2-Hexanone	127.2	Methyl butyl ketone
ketone	2,4-Pentanedione	140.6	Acetylacetone
ketone	4-Heptanone	143.7	Dipropyl ketone
ketone	3-Heptanone	147.8	Ethyl butyl ketone
ketone	2-Heptanone	151	Methyl pentyl ketone
ketone	Cyclohexanone	155.7	J 1 J
ketone	2,6-Dimethyl-4-heptanone	168.1	Diisobutyl ketone
ketone	4-Hydroxy-4-methyl-2-pentanone	169.2	,
ketone	2,5-Hexanedione	191.4	
ketone	Acetophenone	202.1	Methyl phenyl ketone
ketone	Camphor	207	1,7,7-Trimethylbicyclo- [2.2.1] heptan-2-one
ketone	Isophorone	215.2	3,5,5-Trimethylcyclo- hex-2-en-1-one
miscellaneous	Carbon disulfide	46.3	
miscellaneous	Tributyl borate	238.5	
nitrile	Acetonitrile	81.6	
nitrile	Benzonitrile	191.0	Cyanobenzene
nitrile	Phenylacetonitrile	233.5	Cyanomethylbenzene
nitro compound	Nitromethane	101.2	
nitro compound	Nitroethane	114.1	
nitro compound	2-Nitropropane	120.3	Nitroisopropane
nitro compound	1-Nitropropane	131.2	* *
nitro compound	Nitrobenzene	210.8	
nitro compound	1-Methoxy-2-nitrobenzene	277	
sulfide	Thiophene	84.2	
sulfoxide	Dimethylsulfoxide	189.0	DMSO

TABLE 4.6 Molecular Elevation of the Boiling Point

Ebullioscopic constants

Molecular weights can be determined with the relation

$$M = K_b \frac{1000 w_2}{w_1 \Delta T_b}$$

where ΔT_b is the elevation of the boiling point brought about by the addition of w_2 grams of solute to w_1 grams of solvent and K_b is the ebullioscopic constant. In the column headed "Barometric correction" is given the number of degrees for each millimeter of difference between the barometric reading and 760 mmHg to be subtracted from K_b if the pressure is lower, or added if higher, than 760 mm. In general, the effect is within experimental error if the pressure is within 10 mm of 760 mm.

	Barometric	
Compound	correction	K_b
Acetic acid	0.000 8	3.07
Acetic anhydride		3.53
Acetone	0.0004	1.71
Acetonitrile		1.30
Acetophenone		5.65
Aniline	0.0009	3.52
Benzene	0.0007	2.53
Benzonitrile		3.87
Bromobenzene	0.001 6	6.26
Bromoethane		2.53
2-Butanone		2.28
cis-2-Butene-1,4-diol		2.86
D-(+)-Camphor	0.001 5	5.611
Carbon disulfide	0.0006	2.34
Carbon tetrachloride	0.001 3	5.03
Chlorobenzene	0.001 1	4.15
Chloroethane		1.95
Chloroform	0.0009	3.63
Cyclohexane	0.0007	2.79
1,2-Dibromoethane	0.001 6	6.608
1,1-Dichloroethane		3.13
1,2-Dichloroethane		3.44
Dichloromethane		2.60
Diethyl ether	0.000 5	2.02
Diethyl sulfide		3.23
Dimethoxymethane		2.125
N,N-Dimethylacetamide		3.22
Dimethyl sulfide		1.85
1.4-Dioxane		3.270
Ethanol	0.000 3	1.22
Ethoxybenzene		5.0
Ethyl acetate	0.0007	2.77
Formic acid		2.4
Glycerol		6.52
Heptane	0.000 8	3.43
Hexane		2.75
2-Hydroxybenzaldehyde		4.96

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TABLE 4.6 Molecular Elevation of the Boiling Point (*continued*)

	Barometric	
Compound	correction	K_b
Iodoethane		5.16
Iodomethane		4.19
4-Isopropyl-1-methylbenzene		5.52
Methanol	0.000 2	0.83
Methoxybenzene		4.502
Methyl acetate	0.000 5	2.15
2-Methyl-2-butanol		2.255
3-Methyl-1-butanol		2.65
3-Methylbutyl acetate		4.83
Methyl formate		1.649
2-Methyl-1-propanol		2.166
2-Methyl-2-propanol		1.745
Naphthalene	0.001 4	5.80
Nitrobenzene		5.24
Nitroethane		2.60
Nitromethane		1.86
Octane		4.02
Pentyl acetate		4.83
Phenol	0.0009	3.60
Piperidine		2.84
1-Propanol		1.59
Propionic acid		3.51
Propionitrile		1.87
Pyridine		2.710
Quinoline		5.84
1,1,2,2-Tetrachloroethylene		5.50
1,2,3,4-Tetrahydronaphthalene		5.582
Toluene	0.000 8	3.33
<i>p</i> -Toluidine		4.14
Trichloroethylene		4.43
1,1,2-Trichloro-1,2,2-trifluoroethane		5.75
Triethylamine		3.45
Water	0.000 1	0.512

Distillation is an important historical method for the separation of liquids. A mixture or solution of two liquids is heated until the vapor pressure of the lower boiling compound reaches the pressure of the surroundings. This may be ambient pressure or a lowered pressure caused by application of a vacuum. In either event, vaporization occurs, the vapors are condensed on a cold surface, and the condensed liquid is collected. If the boiling points of the two liquids are sufficiently different given the pressure and efficiency of the apparatus, separation may be achieved. A zeotrope is a mixture that can be separated by distillation.

In contrast, certain mixtures of two (binary) or three (ternary) components form constant boiling mixtures that cannot be separated by distillation. In such cases, each component contributes a fixed amount and the boiling point of the mixture is characteristic of the components. Such a system is called an azeotrope. The boiling point of an azeotrope may be higher or lower than that of the individual components. Common binary azeotropes are listed in Table 4.7 and ternary azeotropes are listed in Table 4.8.

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures *A zeotrope is a mixture that can be separated by distillation.*

A. Binary azeotropes containing water

		Composition	Composition, wt %		
System	BP of azeotrope, °C	Water	Other component		
	Inorganic acids				
Hydrogen bromide	126	52.5	47.5		
Hydrogen chloride	108.58	79.78	20.22		
Hydrogen fluoride	111.35	64.4	35.6		
Hydrogen iodide	127	43	57		
Hydrogen peroxide	zeotrope				
Nitric acid	120.7	32.6	67.4		
Perchloric acid	203	28.4	71.6		
	203	20.4	71.0		
	Organic acids				
Formic acid	107.2	22.6	77.4		
Acetic acid	zeotrope				
Propionic acid	99.9	82.3	17.7		
Isobutyric acid	99.3	79	21		
Butyric acid	99.4	81.6	18.4		
Pentanoic acid	99.8	89	11		
Isopentanoic acid	99.5	81.6	18.4		
Perfluorobutyric acid	97	71	29		
Crotonic acid	99.9	97.8	2.2		
	Alcohols				
	70.17	4	0.6		
Ethanol	78.17	4	96 72.2		
Allyl alcohol	88.9	27.7	72.3		
1-Propanol	71.7	71.7	28.3		
2-Propanol	80.3	12.6	87.4		
1-Butanol	92.7	42.5	57.5		
2-Butanol	87.0	26.8	73.2		
2-Methyl-2-propanol	79.9	11.7	88.3		
1-Pentanol	95.8	54.4	45.6		
2-Pentanol	91.7	36.5	63.5		
3-Pentanol	91.7	36.0	64.0		
2,2-Dimethyl-2-propanol	87.35	27.5	72.5		
1-Hexanol	97.8	67.2	32.8		
1-Octanol	99.4	90	10		
Cyclopentanol	96.25	58	42		
1-Heptanol	98.7	83	17		
Phenol	99.52	90.8	9.2		
2-Methoxyphenol	99.5	87.5	12.5		

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

System	BP of azeotrope,	Composition, wt %	
		Water	Other component
	Alcohols (continued)	
1-Phenylphenol	99.95	98.75	1.25
Benzyl alcohol	99.9	91	9
2,3-Dimethyl-2,			
3-butanediol	zeotrope		
Furfuryl alcohol	98.5	80	20
	Aldehydes		ı
Propionaldehyde	47.5	2	98
Butyraldehyde	68	6	94
Pentanal	83	19	81
Paraldehyde	90	28.5	71.5
Furaldehyde	97.5	65	35
	Amines		
N-Methylbutylamine	82.7	15	85
Furfurylamine	99	74	26
Piperidine	92.8	35	65
Pyridine	93.6	41.3	58.7
2-Methylpyridine	93.5	48	52
3-Methylpyridine	97	60	40
4-Methylpyridine	97.35	62.8	37.2
2,6-Dimethylpyridine	96.02	51.8	48.2
Dibutylamine	97	50.5	49.5
Dihexylamine	99.8	92.8	7.2
Triallylamine	95	38	62
Tributylamine	99.65	79.7	20.3
Aniline	98.6	80.8	19.2
N-Ethylaniline	99.2	83.9	16.1
1-Methyl-2-(2-pyridyl)			
pyrrolidine	99.85	97.5	2.5
	Halogenated hydrocarb	oons	
Chloroform	56.1	2.8	97.2
Carbon tetrachloride	42.6	2.8	97.2
Trichloroethylene	73.4	17	83
Tetrachloroethylene	88.5	17.2	82.8
1,2-Dichloroethane	72	8.3	91.7
1-Chloropropane	44	2.2	97.8
1,2-Dichloropropane	78	12	88
Chlorobenzene	90.2	28.4	71.6

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
	Esters		1
Ethyl formate	52.6	5	95
Isopropyl formate	65.0	3	97
Propyl formate	71.6	2.3	97.7
Isobutyl formate	80.4	7.8	92.2
Butyl formate	83.8	14.5	85.5
Isopentyl formate	90.2	21	79
Pentyl formate	91.6	28.4	71.6
Benzyl formate	99.2	80	20
Ethyl acetate	70.38	8.47	91.53
Allyl acetate	83	14.7	85.3
Isopropyl acetate	76.6	10.6	89.4
Propyl acetate	87.4	16.5	83.5
Isobutyl acetate	82.4	14	86
Butyl acetate	90.2	28.7	71.3
Isopentyl acetate	93.8	36.3	63.7
Pentyl acetate	95.2	41	59
Hexyl acetate	97.4	61	39
Phenyl acetate	98.9	75.1	24.9
Benzyl acetate	99.6	87.5	12.5
Methyl propionate	71.4	3.9	96.1
Ethyl propionate	81.2	10	90
Isopropyl propionate	85.2	19.9	80.1
Propyl propionate	88.9	23	77
Isobutyl propionate	92.75	52.2	47.8
Isopentyl propionate	96.55	48.5	51.5
Methyl butyrate	82.7	11.5	88.5
Ethyl butyrate	87.9	21.5	78.5
Propyl butyrate	94.1	36.4	63.6
Isobutyl butyrate	96.3	46	54
Butyl butyrate	97.2	53	47
Isopentyl butyrate	98.05	63.5	36.5
Methyl isobutyrate	77.7	6.8	93.2
Ethyl isobutyrate	85.2	15.2	84.8
Propyl isobutyrate	92.2	30.8	69.2
Isobutyl isobutyrate	95.5	39.4	60.6
Isopentyl isobutyrate	97.4	56.0	44.0
Methyl isopentanoate	87.2	19.2	80.8
Ethyl isopentanoate	92.2	30.2	69.8
Propyl isopentanoate	96.2	45.2	54.8
Isobutyl isopentanoate	90.2 97.4	55.8	44.2
Isopentyl isopentanoate	98.8	74.1	25.9
130penty1 isopentanoate	70.0	74.1	23.9

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TABLE 4.7 Binary Azeotropic (Constant-Boiling) Mixtures (continued)

		Composition, wt %	
BP of azeotrope, °C	Water	Other component	
Esters (continued	d)		
94.5	40	60	
97.2	54	46	
99.08	79.2	20.8	
99.4	84.0	16.0	
99.7	90.9	9.1	
99.9	94	6	
99.9	95.6	4.4	
99.7	91.3	8.7	
99.9	95.5	4.5	
99.95	97.5	2.5	
99.98	98.0	2.0	
95.2	45.1	54.9	
98.12	75.5	24.5	
		92.8	
98.6	74	26	
93.5	38	62	
99	80	20	
99.7	84.6	15.4	
74.35	22	78	
84.8	20	80	
89.0	25	75	
98.6	73	27	
Ethers		1	
34.6	1.5	98.5	
		98.7	
59.5	4	96	
62.2	4.5	95.5	
76.6	11.9	88.1	
88.6	23	77	
92.9	33	67	
97.4	54	46	
82.6	14.5	85.5	
99.33	96.75	3.25	
95.5	40.5	59.5	
Hydrocarbons			
34.6	1.4	98.6	
		94.4	
		87.1	
78.8	11.1	88.9	
	©C Esters (continued 94.5 97.2 99.08 99.4 99.7 99.9 99.9 99.9 99.9 99.95 99.98 95.2 98.12 71 98.6 93.5 99 99.7 74.35 84.8 89.0 98.6 Ethers 34.6 34.2 59.5 62.2 76.6 88.6 92.9 97.4 82.6 99.33 95.5 Hydrocarbons 34.6 61.6 79.2	Esters (continued) 94.5 97.2 99.08 99.4 99.4 99.7 99.9 99.9 99.9 99.9 99.9	

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Compos	sition, wt %
System	BP of azeotrope, °C	Water	Other component
	Hydrocarbons (contin	ued)	
Nonane	94.8	82	18
Undecane	98.85	96.0	4.0
Dodecane	99.45	98	2
Acrolein	52.4	2.6	97.4
Cyclohexene	70.8	8.93	91.07
Cyclohexane	69.5	8.4	91.6
1-Octene	88.0	28.7	71.3
Benzene	69.25	8.83	91.17
Toluene	84.1	13.5	86.5
Ethylbenzene	92.0	33.0	67.0
m-Xylene	92	35.8	64.2
Isopropylbenzene	95	43.8	56.2
Naphthalene	98.8	84	16
	Ketones		
Acetone	zeotrope		
2-Butanone	73.5	11	89
2-Pentanone	83.3	19.5	80.5
Cyclopentanone	94.6	42.4	57.6
4-Methyl-2-pentanone	87.9	24.3	75.7
2-Heptanone	95	48	52
3-Heptanone	94.6	42.2	57.8
4-Heptanone	94.3	40.5	59.5
4-Hydroxy-4-methyl-2-	71.3	10.5	37.3
pentanone	98.8	87.3	12.7
4-Methyl-3-penten-2-one	91.8	34.8	65.2
	Nitriles		
Acetonitrile	76.5	16.3	83.7
Isobutyronitrile	82.5	23	77
Butyronitrile	88.7	32.5	67.5
Acrylonitrile	70.6	14.3	85.7
	Miscellaneous		1
Hydroxino	120	32.3	(7.7
Hydrazine	-	32.3	67.7
Acetamide	zeotrope	22.6	76.4
Nitromethane	83.59	23.6	76.4
Nitroethane	87.22	28.5	71.5
2,5-Dimethylfuran	77.0	11.7	88.3
Trioxane	91.4	30	70
Carbon disulfide	42.6	2.8	97.2

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TABLE 4.7 Binary Azeotropic (Constant-Boiling) Mixtures (*continued*)

B. Binary azeotropes containing organic acids

		Composition, wt %	
System	BP of azeotrope, °C	Acid	Other component
,	Formic acid		
2-Methylbutane	27.2	4	96
Pentane	34.2	20	80
Hexane	60.6	28	72
Methylcyclopentane	63.3	29	71
Cyclohexane	70.7	70	30
Methylcyclohexane	80.2	46.5	53.5
Heptane	78.2	56.5	43.5
Octane	90.5	63	37
Benzene	71.05	31	69
Toluene	85.8	50	50
o-Xylene	95.5	74	26
m-Xylene	92.8	71.8	28.2
Styrene	97.8	73	27
Iodomethane	42.1	6	94
Chloroform	59.15	15	85
Carbon tetrachloride	66.65	18.5	81.5
Trichloroethylene	74.1	25	75
Tetrachloroethylene	88.2	50	50
Bromoethane	38.2	3	97
1.2-Dibromoethane	94.7	51.5	48.5
1,2-Dichloroethane	77.4	14	86
1-Bromopropane	64.7	27	73
2-Bromopropane	77.4	14	86
1-Chloropropane	45.6	8	92
2-Chloropropane	34.7	1.5	98.5
1-Chloro-2-methylpropane	63.0	19	81
Bromobenzene	98.1	68	32
Chlorobenzene	93.7	59	41
Fluorobenzene	73.0	27	73
o-Chlorotoluene	100.2	83	17
Pyridine	127.43	61.4	38.6
2-Methylpyridine	158.0	25	75
2-Pentanone	105.3	32	68
3-Pentanone	105.4	33	67
Nitromethane	97.07	45.5	54.5
Diethyl sulfide	82.2	35	65
Diisopropyl sulfide	93.5	62	38
Dipropyl sulfide	98.0	83	17
Carbon disulfide	42.55	17	83

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composit	tion, wt %
System	BP of azeotrope, °C	Acid	Other component
	Acetic acid		
Hexane	68.3	6.0	94.0
Heptane	91.7	23	67
Octane	105.7	53.7	46.3
Nonane	112.9	69	31
Decane	116.75	79.5	20.5
Undecane	117.9	95	5
Cyclohexane	78.8	9.6	90.4
Methylcyclohexane	96.3	31	69
Benzene	80.05	2.0	98.0
Toluene	100.6	28.1	71.9
o-Xylene	116.6	78	22
m-Xylene	115.35	72.5	27.5
p-Xylene	115.25	72	28
Ethylbenzene	114.65	66	34
Styrene	116.8	85.7	14.3
Isopropylbenzene	116.0	84	16
Triethylamine	163	67	33
Nitromethane	101.2	96	4
Nitroethane	112.4	30	70
Pyridine	138.1	51.1	48.9
2-Methylpyridine	144.1	40.4	59.6
3-Methylpyridine	152.5	30.4	69.6
4-Methylpyridine	154.3	30.3	69.7
2,6-Dimethylpyridine	148.1	22.9	77.1
Carbon tetrachloride	76	98.46	1.54
Trichloroethylene	86.5	96.2	3.8
Tetrachloroethylene	107.4	61.5	38.5
1,2-Dibromoethane	114.4	55	45
2-Iodopropane	88.3	9	91
1-Bromobutane	97.6	18	82
1-Bromo-2-methylpropane	90.2	12	88
Chlorobenzene	114.7	58.5	41.5
Trichloronitromethane	107.65	80.5	19.5
1,4-Dioxane	119.5	77	23
Diisopropyl sulfide	111.5	48	52
	Propanoic (Propionic)	acid	
Heptane	97.8	2	98
Octane	120.9	21.5	78.5

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Compositi	ion, wt %
System	BP of azeotrope, °C	Acid	Other component
	Acetic acid (continu	ued)	
Nonane	134.3	54.0	46.0
Decane	139.8	80.5	19.5
o-Xylene	135.4	43	57
<i>p</i> -Xylene	132.5	34	66
1,3,5-Trimethylbenzene	139.3	77	23
Isopropylbenzene	139.0	65	35
Propylbenzene	139.5	75	25
Camphene	138.0	65	35
α-Pinene	136.4	58.5	41.5
Methoxybenzene	140.8	96	4
Pyridine	148.6	67.2	32.8
2-Methylpyridine	154.5	55.0	45.0
1,2-Dibromoethane	127.8	17.5	82.5
1-Iodo-2-methylpropane	119.5	9	91
Chlorobenzene	128.9	18	82
Dipropyl sulfide	136.5	45	55
2 ipropyr sumae			
	Butyric (butanoic) a	acid	
Undecane	162.4	84.4	15.5
o-Xylene	143.0	10	90
m-Xylene	138.5	6	94
<i>p</i> -Xylene	137.8	5.5	94.5
Ethylbenzene	135.8	4	96
Styrene	143.5	15	85
1,2,4-Trimethylbenzene	159.5	45	55
1,3,5-Trimethylbenzene	158.0	38	62
Isopropylbenzene	149.5	20	80
Propylbenzene	154.5	28	72
Butylbenzene	162.5	75	25
Naphthalene	zeotrope		
Indene	163.7	84	16
Camphene	152.3	2.8	97.2
Methoxybenzene	152.9	12	88
Pyridine	163.2	92.0	8.0
2-Furaldehyde	159.4	42.5	57.5
1,2-Dibromoethane	131.1	3.5	96.5
1-Iodobutane	129.8	2.5	97.5
Chlorobenzene	131.75	2.8	97.2
1,4-Dichlorobenzene	162.0	57	43
o-Bromotoluene	163.0	72	28
m-Bromotoluene	163.6	79.5	20.5
p-Bromotoluene	161.5	75	25
α -Chlorotoluene	160.8	65	35
Ethyl bromoacetate	157.4	84	16
Propyl chloroacetate	160.5	40	60

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composi	Composition, wt%	
System	BP of azeotrope, °C	Acid	Other component	
	Isobutyric (2-methylpropa	noic) acid		
2,7-Dimethyloctane	148.6	48	52	
o-Xylene	141.0	22	78	
m-Xylene	139.9	15	85	
p-Xylene	136.4	13	87	
Styrene	142.0	27	73	
1,2,4-Trimethylbenzene	152.3	63	37	
Isopropylbenzene	146.8	35	65	
Propylbenzene	149.3	49	51	
Camphene	148.1	45	55	
D-Limonene	152.5	78	22	
Methoxybenzene	149.0	42	58	
Ethyl bromoacetate	153.0	40	60	
Ethyl 2-oxopropionate	153.0	60	40	
1,2-Dibromoethane	130.5	6.5	93.5	
1-Iodobutane	128.8	7	93	
1-Bromohexane	148.0	35	65	
Bromobenzene	148.6	35	65	
Chlorobenzene	131.5	8	92	
o-Bromotoluene	153.9	85	15	
α-Chlorotoluene	153.5	80	20	
Diisopentyl ether	154.2	93	7	
Ethyl bromoacetate	153.0	40	60	

C. Binary azeotropes containing alcohol

		Composition, wt %	
System	BP of azeotrope, °C	Alcohol	Other component
	Methanol		
Pentane	30.9	7	93
Cyclopentane	38.8	14	86
Cyclohexane	53.9	36.4	63.6
Methylcyclohexane	59.2	54	46
Heptane	59.1	51.5	48.5
Octane	62.8	67.5	32.5
Nonane	64.1	83.4	16.6
Benzene	57.5	39.1	60.9
Fluorobenzene	59.7	32	68
Toluene	63.5	72.5	27.5
Bromomethane	3.55	99.55	0.45
Iodomethane	37.8	95.5	4.5

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composit	ion, wt %
System	BP of azeotrope, °C	Alcohol	Other component
	Methanol (continue	ed)	
Bromodichloromethane	63.8	60	40
Chloroform	53.4	87.4	12.6
Carbon tetrachloride	55.7	79.44	20.56
Bromoethane	34.9	5.3	94.7
1,2-Dichloroethane	61.0	32	68
Trichloroethylene	59.3	38	62
1-Bromopropane	54.5	21	79
2-Bromopropane	48.6	15.0	85.0
1-Chloropropane	40.5	9.5	90.5
2-Chloropropane	33.4	6	94
2-Iodopropane	61.0	38	62
1-Chlorobutane	57.0	27	73
Isobutyl formate	64.6	95	5
Methyl acetate	53.5	19	81
Methyl acrylate	62.5	54	46
Methyl nitrate	52.5	73	27
Acetone	55.5	12.1	87.9
1,4-Dioxane	zeotrope	12.1	07.7
Dipropyl ether	63.8	72	28
Methyl <i>tert</i> -butyl ether	51.3	14.3	85.7
Diethyl sulfide	61.2	62	38
Carbon disulfide	39.8	71	29
	59.8 59.7	16.4	83.6
Thiophene Nitromethane	59.7 64.4	9.1	83.6 90.9
Nitrometnane	04.4	9.1	90.9
	Ethanol		
Pentane	34.3	5	95
Cyclopentane	44.7	7.5	92.5
Hexane	58.7	21	79
Cyclohexane	64.8	29.2	70.8
Heptane	70.9	49	51
Octane	77.0	78	22
Benzene	67.9	31.7	68.3
Fluorobenzene	70.0	75	25
Toluene	76.7	68	32
Bromodichloromethane	75.5	72	28
Iodomethane	41.2	96.8	3.2
Chloroform	59.3	93	7
Trichloronitromethane	77.5	34	66
Carbon tetrachloride	65.0	84.2	15.8
1,2-Dichloroethane	70.5	37	63
3-Chloro-1-propene	44	5	95
5-Cinoro-1-propene	44	3	93

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composi	tion, wt %
System	BP of azeotrope, °C	Alcohol	Other component
	Ethanol (continue	rd)	
1-Bromopropane	62.8	20.5	79.5
2-Bromopropane	55.6	10.5	89.5
1-Chloropropane	45.0	6	94
2-Chloropropane	35.6	2.8	97.2
1-Iodopropane	75.4	44	56
2-Iodopropane	71.5	27	73
1-Bromobutane	75.0	43	57
1-Chlorobutane	65.7	20.3	79.7
2-Butanone	74.8	40	60
1,1-Diethoxyethane	78.0	76	24
Dipropyl ether	74.5	44	56
Acetonitrile	72.5	44	56
Acrylonitrile	70.8	41	59
Nitromethane	76.1	29	71
Carbon disulfide	42.6	91	9
Diethyl sulfide	72.6	56	44
Hexane	1-Propanol	4	96
Cyclohexane	74.7	18.5	81.5
Methylcyclohexane	87.0	34.7	65.3
Heptane	84.6	34.7	65.3
Octane	93.9	70	30
Benzene	77.1	16.9	83.1
Toluene	92.5	51.2	48.8
o-Xylene	zeotrope	31.2	70.0
m-Xylene	97.1	94	6
<i>p</i> -Xylene	96.9	92.2	7.8
Styrene	97.0	8	92
Propyl formate	80.7	3	97
Butyl formate	95.5	64	36
Propyl acetate	94.7	51	49
Ethyl propionate	93.4	48	52
Methyl butyrate	94.4	49	51
Dipropyl ether	85.7	30	70
1,1-Diethoxyethane	92.4	37	63
1,4-Dioxane	95.3	55	45
Chloroform	zeotrope		
Carbon tetrachloride	73.4	92.1	7.9
Trichloronitromethane	94.1	58.5	41.5
Iodoethane	70	93	7
1,2-Dichloroethane	80.7	19	81

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composit	Composition, wt %	
System	BP of azeotrope, °C	Alcohol	Other	
System		Alcohol	componen	
	1-Propanol (continu	ued)		
Tetrachloroethylene	94.0	52	48	
1-Bromopropane	69.7	9	91	
1-Chlorobutane	74.8	18	82	
Chlorobenzene	96.5	80	20	
Fluorobenzene	80.2	18	82	
Nitromethane	89.1	48.4	51.6	
1-Nitropropane	97.0	8.8	91.2	
Carbon disulfide	45.7	94.5	5.5	
<u> </u>	2-Propanol			
Pentane	35.5	6	94	
Hexane	62.7	23	77	
Cyclohexane	69.4	32	68	
Heptane	76.4	50.5	49.5	
Octane	81.6	84	16	
Benzene	71.7	33.7	66.3	
Fluorobenzene	74.5	30	70	
Toluene	80.6	69	31	
Chloroform	60.8	4.2	95.8	
Trichloronitromethane	81.9	35	65	
Carbon tetrachloride	69.0	18	82	
1,2-Dichloroethane	74.7	43.5	56.5	
Iodoethane	67.1	15	85	
3-Bromo-1-propene	66.5	20	80	
1-Chloropropane	46.4	2.8	97.2	
1-Bromopropane	66.8	20.5	79.5	
2-Bromopropane	57.8	12	88	
1-Iodopropane	79.8	42	58	
2-Iodopropane	76.0	32	68	
1-Chlorobutane	70.8	23	77	
Ethyl acetate	75.3	25	75	
Isopropyl acetate	81.3	60	40	
Methyl propionate	76.4	37	63	
Acrylonitrile	71.7	56	44	
Butylamine	74.7	60	40	
2-Butanone	77.5	32	68	
1,1-Diethoxyethane	81.3	63	37	
Ethyl propyl ether	62.0	10	90	
Diisopropyl ether	66.2	14.1	85.9	

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composi	tion, wt %
System	BP of azeotrope, °C	Alcohol	Other component
	1-Butanol		
Cyclohexane	79.8	9.5	90.5
Cyclohexene	82.0	5	95
Hexane	68.2	3.2	96.8
Methylcyclohexane	95.3	20	80
Heptane	93.9	18	82
Octane	108.5	45.2	54.8
Nonane	115.9	71.5	28.5
Toluene	105.5	27.8	72.2
o-Xylene	116.8	75	25
m-Xylene	116.5	71.5	28.5
p-Xylene	115.7	68	32
Ethylbenzene	115.9	65.1	34.9
Butyl formate	105.8	23.6	76.4
Isopentyl formate	115.9	69	31
Butyl acetate	117.2	47	53
Isobutyl acetate	114.5	50	50
Ethyl butyrate	115.7	64	36
Ethyl isobutyrate	109.2	17	83
Methyl isopentanoate	113.5	40	60
Ethyl borate	113.0	52	48
Ethyl carbonate	116.5	63	37
Isobutyl nitrate	112.8	45	55
Dibutyl ether	117.8	82.5	17.5
Diisobutyl ether	113.5	48	52
1,1-Diethoxyethane	101.0	13	87
Carbon tetrachloride	76.6	97.6	2.4
Tetrachloroethylene	110.0	68	32
2-Bromo-2-methylpropane	90.2	7	93
2-Iodo-2-methylpropane	110.5	30	70
Chlorobenzene	115.3	56	44
		52	48
Paraldehyde	115.8		22.9
Hexaldehyde Ethylenediamine	116.8 124.7	77.1 35.7	64.3
Pyridine Pyridine	118.6	69	31
1-Nitropropane	115.3	32.2	67.8
Butyronitrile	113.0	50	50
•			
Diisopropyl sulfide	112.0	45	55
	2-Methyl-2-propa	nol	I
Cyclohexene	80.5	14.2	85.8
Cyclohexane	78.3	14	86

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composition, wt %	
System	BP of azeotrope, °C	Water	Other component
	2-Methyl-2-propanol (co	ontinued)	
Methylcyclopentane	71.0	5	95
Hexane	68.3	2.5	97.5
Methylcyclohexane	92.6	32	68
Heptane	90.8	27	73
2,5-Dimethylhexane	98.7	42	58
1,3-Dimethylcyclohexane	102.2	56	44
2,2,4-Trimethylpentane	92.0	27	73
Benzene	79.3	7.4	92.6
Chlorobenzene	107.1	63	37
Fluorobenzene	84.0	9	91
Toluene	101.2	45	55
Ethylbenzene	107.2	80	20
p-Xylene	107.1	88.6	11.4
Butyl formate	103.0	40	60
Isobutyl formate	97.4	12	88
Propyl acetate	101.0	17	83
Isobutyl acetate	107.6	92	8
Methyl butyrate	101.3	25	75
Ethyl isobutyrate	105.5	52	48
Methyl chloroacetate	107.6	12	88
Dipropyl ether	89.5	10	90
	82.7	6.2	93.8
Isobutyl vinyl ether	82.7 98.2	20	
1,1-Diethoxyethane		19	80
2-Pentanone	101.8		81
3-Pentanone	107.7	20	80
1,2-Dichloroethane	83.5	6.5	93.5
1-Bromobutane	95.0	21	79
1-Chlorobutane	77.7	4	96
2-Bromo-2-methylpropane	88.8	12	88
2-Iodo-2-methylpropane	104.0	36	64
1-Nitropropane	105.3	15.2	84.8
Isobutyl nitrate	105.6	36	64
Diisopropyl sulfide	105.8	73	27
	3-Methyl-1-butan	iol	
Heptane	97.7	7	93
Octane	117.0	30	70
Гoluene	109.7	10	90
Ethylbenzene	125.7	49	51
Isopropylbenzene	131.6	94	6
Camphene	130.9	24	76

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

BP of azeotrope.		
BP of azeotrope, °C	Alcohol	Other component
3-Methyl-1-butanol (co	ntinued)	
131.7	85	15
112.1	14.0	86.0
125.9	16.5	83.5
123.5	22.0	78.0
129.8	65	35
Cyclohexanol		
143.0	14	86
138.9	5	95
153.8	40	60
160.0	75	25
151.9	41	59
160.6	92	8
Allyl alcohol	I	
85.0	42	58
	4.5	95.5
	1	42
		50
93.4	68	32
		82.64
		50
		47
		45
		82
	_	72
		15
85.1	45	55
Phenol	1	I
159.5	6	94
	35	65
		16.9
		54
		75
		79
		53
		78
		49.0
	131.7 112.1 125.9 123.5 129.8 Cyclohexanol 143.0 138.9 153.8 160.0 151.9 160.6 Allyl alcohol 85.0 65.5 74.0 89.3 93.4 76.75 92.4 94.2 93.8 79.9 89.4 96.2 85.1	112.1 14.0 125.9 16.5 123.5 22.0 129.8 65 Cyclohexanol 143.0 14 138.9 5 153.8 40 160.0 75 151.9 41 160.6 92 Allyl alcohol 85.0 42 45 68 76.75 17.36 92.4 50 93.4 68 76.75 17.36 92.4 50 94.2 53 93.8 55 79.9 18 89.4 28 96.2 85 85.1 45 Phenol 159.5 6 168.0 35 180.6 83.1 175.0 46 166.0 25 163.5 21 177.8 47 156.1 22

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composi	tion, wt %	
System	BP of azeotrope, °C	Alcohol	Other component	
	Phenol (continue	d)		
1-Octanol	195.4	13	87	
2-Octanol	184.5	50	50	
Dipentyl ether	180.2	78 22		
Diisopentyl ether	172.2	15	85	
2-Methylpyridine	185.5	75.4	24.6	
3-Methylpyridine	188.9	71.2	29.8	
	190.0	67.5	32.5	
	193.4	57.0	43.0	
		72.5	27.5	
		52.3	47.7	
Aniline		41.9	58.1	
Ethylene diacetate 195.5		39.2	60.8	
odobenzene 177.7		53	47	
	Benzyl alcohol			
N	204.1	(0)	40	
		60		
		11	89	
		57	43	
			20	
		61	39 38 70 93.5	
p-Cresol		62		
N-Methylaniline		30		
		6.5		
		50	50	
		72	28	
Iodobenzene		12	88	
Nitrobenzene	204.0	58	42	
o-Bromotoluene	181.3	7	93	
Borneol	205.1	85.8	14.2	
	2-Ethoxyethano	1		
Methylcyclohexane	98.6	15	85	
Heptane	96.5	14	86	
Octane	116.0	38	62	
Toluene	110.2	10.8	89.2	
Ethylbenzene	127.8	48	52	
p-Xylene	128.6	50	50	
Styrene	130.0	55	45	
Propylbenzene	134.6	80	20	
Isopropylbenzene	133.2	67	33	
Camphene	131.0	65	35	
Dectanol 184.5 180.2 180.2 180.2 180.2 180.2 180.2 185.5 Methylpyridine 185.5 Methylpyridine 190.0		72	28	

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composit	ion, wt %
System	BP of azeotrope, °C	Alcohol	Other component
	2-Butoxyethano	ol	
Dipentene	164.0	53	47
1,3,5-Trimethylbenzene	162.0	32	68
Butylbenzene	169.6	73.4	26.6
Camphene	154.5	30	70
o-Cresol	191.6	15	85
Phenetole	167.1	52	48
Cineole	168.9	58.5	41.5
Benzaldehyde	171.0	91	9
Diisobutyl sulfide	163.8	42	58
I	1,2-Ethanedio	<u> </u> 	
Heptane	97.9	3	97
Decane		23	77
Tridecane	161.0 188.0	55	77 45
Toluene	110.1	2.3	97.7
Styrene	139.5	16.5	83.5
Stilbene	196.8	87	13
m-Xylene	135.1	6.55	93.45
p-Xylene	134.5	6.4	93.6
1,3,5-Trimethylbenzene	156	13	87
Propylbenzene	152	19	81
Isopropylbenzene	147.0	18	82
Naphthalene	183.9	51	49
1-Methylnaphthalene	190.3	60.0	40.0
2-Methylnaphthalene	189.1	57.2	42.8
Anthracene	197	98.3	1.7
Indene	168.4	26	74
Acenaphthene	194.65	74.2	25.8
Fluorene	196.0	82	18
Camphene	152.5	20	80
Camphor	186.2	40	60
Biphenyl	192.3	66.5	33.5
Diphenylmethane	193.3	68.5	31.5
Benzyl alcohol	193.1	56	44
2-Phenylethanol	194.4	69	31
o-Cresol	189.6	27	73
m-Cresol	195.2	60	40
3,4-Dimethylphenol	197.2	89	11
Menthol	188.6	51.5	48.5
Ethyl benzoate	186.1	46.5	53.5
o-Bromotoluene	166.8	25	75
Dibutyl ether	139.5	6.4	93.6

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

		Composi	tion, wt %	
System	BP of azeotrope, °C	Alcohol	Other component	
	1,2-Ethanediol (conti	inued)		
Methoxybenzene	150.5	10.5	89.5	
Diphenyl ether	193.1	60	40	
Benzyl phenyl ether	195.5		13	
Acetophenone	185.7	52	48	
2,4-Dimethylaniline	188.6	47	53	
N,N-Dimethylaniline	175.9	33.5	66.5	
m-Toluidine	188.6	42	58	
2,4,6-Trimethylpyridine 170.5		9.7	90.3 20.5	
Quinoline	line 196.4			
Tetrachloroethylene	119.1	94	6 96	
1,2-Dibromoethane	129.8	4		
Chlorobenzene	130.1	94.4	5.6	
α-Chlorotoluene	167.0	30	70	
Nitrobenzene	185.9	59	41	
o-Nitrotoluene	188.5	48.5	51.5	
	1,2-Ethanediol monoa	acetate		
Indene	180.0	20	80	
1-Octanol	189.5	71	29	
Phenol	197.5	65	35	
o-Cresol	199.5	51	49	
m-Cresol	206.5	31	69	
p-Cresol	206.0	33	67	
Dipentyl ether	180.8	42	58	
Diisopentyl ether	170.2	28	72	
m-Bromotoluene	182.0	32 68		

D. Binary azeotropes containing ketones

		Composi	tion, wt %
System	BP of azeotrope, °C	Ketone	Other component
	Acetone		
Cyclopentane	41.0	36	64
Pentane	32.5	20	80
Cyclohexane	53.0	67.5	32.5
Hexane	49.8	59	41

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Compositi	on, wt %	
System	BP of azeotrope, °C	Ketone	Other component	
	Acetone (continue	ed)		
Heptane	55.9	89.5	10.5	
Diethylamine	51.4	38.2	61.8	
Methyl acetate	55.8	48.3	51.7	
Diisopropyl ether	54.2	61	39	
Chloroform	64.4	78.1	21.9	
Carbon tetrachloride	56.1	11.5	88.5	
Carbon disulfide	39.3	67	33	
Ethylene sulfide	51.5	57	43	
	2-Butanone			
Cyclohexane	71.8	40	60	
Hexane	64.2	28.6	71.4	
Heptane	77.0	70	30	
2,5-Dimethylhexane	79.0	95	5	
Benzene	78.33	44	56	
2-Methyl-2-propanol	78.7	69	31	
Butylamine	74.0	35	65	
Ethyl acetate	77.1	11.8	88.2	
Methyl propionate	79.0	60	40	
Butyl nitrite	76.7	30	70	
1-Chlorobutane	77.0	38	62	
Fluorobenzene	79.3	75	25	

E. Miscellaneous binary azeotropes

		Composition, wt %		
System	BP of azeotrope, °C	Solvent	Other component	
	Solvent: acetamic	le		
Dipentene	169.2	18	82	
Biphenyl	213.0	50.5	49.5	
Diphenylmethane	215.2	56.5	43.5	
1,2-Diphenylethane	218.2	68	32	
o-Xylene	142.6	11	89	
m-Xylene	138.4	10	90	
p-Xylene	137.8	8	92	
Styrene	144	12	88	
4-Isopropyl-1-				
methylbenzene	170.5	19	81	

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TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

		Composi	tion, wt %
System	BP of azeotrope, °C	Solvent	Other component
	Solvent: acetamide (con	ntinued)	
Naphthalene	199.6	27	73
1-Methylnaphthalene	209.8	43.8	56.2
2-Methylnaphthalene	208.3	40	60
Indene	177.2	17.5	82.5
Acenaphthene	217.1	64.2	35.8
Camphene	155.5	12	88
Camphor	199.8	23	77
Benzaldehyde	178.6	6.5	93.5
3,4-Dimethylphenol	221.1	96	4
2-Methoxy-4-(2-propenyl)-			
phenol	220.8	88	12
N-Methylaniline	193.8	14	86
N-Ethylaniline	199.0	18	82
N,N-Diethylaniline	198.1	24	76
Diphenyl ether	214.6	52	48
Safrole	208.8	32	68
Tetrachloroethylene	120.5	97.4	2.6
	Solvent: aniline		
Nonane	149.2	13.5	86.5
Decane	167.3	36	64
Undecane	175.3	57.5	42.5
Dodecane	180.4	71.5	28.5
Tridecane	182.9	86.2	13.8
Tetradecane	183.9	95.2	4.8
Butylbenzene	177.8	46	54
1,2,4-Trimethylbenzene	168.6 164.3	13.5 12.0	86.5 88.0
1,3,5-Trimethylbenzene Indene	164.3 179.8	41.5	88.0 58.5
1-Octanol	183.9	83	17
o-Cresol	191.3	8	92
Dipentyl ether	177.5	55	45
Diisopentyl ether	169.3	28	72
Hexachloroethane	176.8	66	34
Trexacinoroculaile	170.0	00	31
	Solvent: pyridine	2	I
Heptane	95.6	25.3	74.7
Octane	109.5	56.1	43.9
Nonane	115.1	89.9	10.1
Toluene	110.1	22.2	77.8
Phenol	183.1	13.1	86.9
Piperidine	106.1	8	92

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

Solvent 14 41.2 11.2 83.2 64 42.7 ne 16 64.7 51.9 4.7 99.3	86 58.8 88.8 16.8 36 57.3
14 41.2 11.2 83.2 64 42.7 ne 16 64.7 51.9 4.7	58.8 88.8 16.8 36 57.3
41.2 11.2 83.2 64 42.7 me 16 64.7 51.9 4.7	58.8 88.8 16.8 36 57.3
11.2 83.2 64 42.7 me 16 64.7 51.9 4.7	88.8 16.8 36 57.3
83.2 64 42.7 me 16 64.7 51.9 4.7	16.8 36 57.3
64 42.7 ne 16 64.7 51.9 4.7	36 57.3
42.7 16 64.7 51.9 4.7	57.3
16 64.7 51.9 4.7	84
16 64.7 51.9 4.7	
64.7 51.9 4.7	
51.9 4.7	25.2
4.7	33.3
1	48.1
99.3	95.3
	0.7
46.3	53.7
78.8	21.2
48.3	51.7
97.7	2.3
ethyl) ether	
48	52
52	48
22	78
22	78
45	55
39	61
	38
1	20
7	93
18	82
10	90
96.3	3.7
	85
13	87
	54
	67
46	54
	20
	90
	75
	89.5
	71
	87
	62 80 7 18 10 96.3 15

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 TABLE 4.8
 Ternary Azeotropic Mixtures

A. Ternary azeotropes containing water and alcohols

	DD C	Co	omposition, v	wt %
System	BP of azeotrope, °C	Water	Alcohol	Other component
	Methanol			
Chloroform	52.3	1.3	8.2	90.5
2-Methyl-1,3-butadiene	30.2	0.6	5.4	94.0
Methyl chloroacetate	67.9	6.3	81.2	13.5
	Ethanol			
Acetonitrile	72.9	1	55	44
Acrylonitrile	69.5	8.7	20.3	71.0
Benzene	64.9	7.4	18.5	74.1
Butylamine	81.8	7.5	42.5	50.0
Butyl methyl ether	62	6.3	8.6	85.1
Carbon disulfide	41.3	1.6	5.0	93.4
Carbon tetrachloride	62	4.5	10.0	85.5
Chloroform	55.3	2.3	3.5	94.2
Crotonaldehyde	78.0	4.8	87.9	7.3
Cyclohexane	62.6	4.8	19.7	75.5
1,2-Dichloroethane	66.7	5	17	78
1,1-Diethoxyethane	77.8	11.4	27.6	61.0
Diethoxymethane	73.2	12.1	18.4	69.5
Ethyl acetate	70.2	9.0	8.4	82.6
Heptane	68.8	6.1	33.0	60.9
Hexane	56.0	3	12	85
Toluene	74.4	12	37	51
Trichloroethylene	67.0	5.5	16.1	78.4
Triethylamine	74.7	9	13	78
	1-Propanol			
Dangana	67	7.6	10.1	82.3
Benzene Carbon tetraebleride	65.4	5	10.1	82.3
Carbon tetrachloride Cyclohexane	65.4	8.5	10.0	84 81.5
•	87.6	27.4	51.6	21.0
1,1-Dipropoxyethane				
Dipropoxymethane	86.4 74.8	8.0 11.7	44.8 20.2	47.2 68.1
Dipropyl ether			20.2	60
3-Pentanone	81.2 82.5	20		73.0
Propyl acetate	82.5 70.8	17.0 13	10.0	82
Propyl formate Tetrachloroethylene	70.8 81.2	12.5	5 20.7	66.8
	01.2	12.3	20.7	00.8
	2-Propanol			
Benzene	66.5	7.5	18.7	73.8
Butylamine	83	12.5	40.5	47.0

TABLE 4.8 Ternary Azeotropic Mixtures (*continued*)

System 2-Pro Cyclohexane Toluene Trichloroethylene Butyl acetate Butyl formate Dibutyl ether	BP of azeotrope, °C panol (continued 64.3 76.3 69.4 1-Butanol	7.5 13.1 7	18.5 38.2 20	74.0 48.7 73
Cyclohexane Toluene Trichloroethylene Butyl acetate Butyl formate	64.3 76.3 69.4 1-Butanol	7.5 13.1 7	38.2	48.7
Toluene Trichloroethylene Butyl acetate Butyl formate	76.3 69.4 1-Butanol	13.1	38.2	48.7
Butyl acetate Butyl formate	69.4 1-Butanol	7		
Butyl formate	89.4			
Butyl formate				
		37.3	27.4	35.3
Dibutyl ether	83.6	21.3	10.0	68.7
	90.6	29.9	34.6	35.5
Heptane	78.1	41.4	7.6	51.0
Hexane	61.5	19.2	2.9	77.9
Nonane	90.0	69.9	18.3	11.8
Octane	86.1	60.0	14.6	25.4
	2-Butanol			
Carbon tetrachloride	65	4.05	4.95	91.00
Cyclohexane	69.7	8.9	10.8	80.3
Isooctane	76.3	9	19	72
2-M	ethyl-1-propanol			
Isobutyl acetate	86.8	30.4	23.1	46.5
Isobutyl formate	80.2	17.3	6.7	76.0
Toluene	81.3	17.9	16.4	65.7
2-M	ethyl-2-propanol			
Benzene	67.3	8.1	21.4	70.5
Carbon tetrachloride	64.7	3.1	11.9	85.0
Cyclohexane	65.0	8	21	71
3-M	lethyl-1-butanol		'	
Isopentyl acetate	93.6	44.8	31.2	24.0
Isopentyl formate	89.8	32.4	19.6	48.0
	Allyl alcohol		'	
Benzene	68.2	8.6	9.2	82.2
Carbon tetrachloride	65.2	5	11	84
Cyclohexane	66.2	8	11	81
Hexane	59.7	8.5	5.1	86.4

TABLE 4.8 Ternary Azeotropic Mixtures (continued) B. Other ternary azeotropes

System	BP of azeotrope, °C	Composition, wt %	System	BP of azeotrope, °C	Composition, wt %
Water Acetone 2-Methyl-1,3-butadiene	32.5	0.4 7.6 92.0	Water Nitromethane Heptane	71.4	7.9 29.7 62.4
Water Acetonitrile Benzene	66	8.2 23.3 68.5	Water Nitromethane Nonane	80.7	17.4 58.3 24.3
Water Acetronitrile Trichloroethylene	67	6.4 20.5 73.1	Water Nitromethane Octane	77.4	12.4 44.3 43.3
Water Acetonitrile Triethylamine	68.6	3.5 9.6 86.9	Water Nitromethane Pentane	33.1	2.1 6.5 91.4
Water 2-Butanone Cyclohexane	63.6	5 35 60	Water Nitromethane Undecane	82.8	20.6 73.3 6.1
Water Butyraldehyde Hexane	55.0	4 21 75	Water Pyridine Dodecane	93.5	40.5 54.5 5.0
Water Formic acid Isopentanoic acid	107.6	21.3 76.3 2.4	Water Pyridine Undecane	93.1	38.5 51.0 10.5
Water Formic acid Isobutyric acid	107.0	15.5 66.8 17.7	Water Pyridine Decane	92.3	35.5 45.5 19.0

	Water Formic acid Butyric acid	107.6	19.5 75.9 4.6	Water Pyridine Nonane	90.5	30.5 37.0 32.5
	Water Formic acid Propionic acid	107.2	18.6 71.9 9.5	Water Pyridine Octane	86.7	22.4 25.5 52.0
	Water Hydrogen bromide Chlorobenzene	105	11.0 10.4 78.6	Water Pyridine Heptane	78.6	14.0 15.5 70.5
	Water Hydrogen chloride Chlorobenzene	96.9	20.2 5.3 74.5	Acetic acid Pyridine Acetic anhydride	134.4	23 55 22
	Water Hydrogen chloride Phenol	107.3	64.8 15.8 19.4	Acetic acid Pyridine Decane	134.1	31.4 38.2 30.4
	Water Hydrogen fluoride Fluorosilic acid	116.1	54 10 36	Acetic acid Pyridine Ethylbenzene	129.1	13.5 25.2 61.3
	Water Nitroethane Heptane	75.1	11.5 75.1 64.0	Acetic acid Pyridine Heptane	98.5	3.4 10.6 86.0
	Water Nitroethane Hexane	59.5	8.4 9.3 82.3	Acetic acid Pyridine Nonane	128.0	20.7 29.4 49.9
	Water Nitromethane Decane	82.4	19.1 68.1 12.8	Acetic acid Pyridine Octane	115.7	10.4 20.1 69.5
4	Water Nitromethane Dodecane	83.1	21.5 75.3 3.2	Acetic acid Pyridine o-Xylene	132.2	17.7 30.5 51.8

TABLE 4.8 Ternary Azeotropic Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt%	System	BP of azeotrope, °C	Composition, wt%
Acetic acid Pyridine p-Xylene	129.2	10.2 22.5 67.3	Methanol Methyl acetate Hexane	47.4	14.6 36.8 48.6
Acetic acid 2,6-Dimethylpyridine Undecane	163.0	75.0 13.8 11.2	Ethanol Acetone Chloroform	63.2	10.4 24.3 65.3
Acetic acid 2,6-Dimethylpyridine Decane	147.0	12.6 74.3 13.1	Ethanol Acetonitrile Triethylamine	70.1	8 34 58
Acetic acid 2-Methylpyridine Decane	141.3	19.9 46.8 33.3	Ethanol Benzene Cyclohexane	64.7	29.6 12.8 57.6
Acetic acid 2-Methylpyridine Nonane	135.0	12.8 38.4 48.8	Ethanol Chloroform Hexane	57.3	9.5 56.1 34.4
Acetic acid 2-Methylpyridine Octane	121.3	3.6 24.8 71.6	1-Propanol Benzene Cyclohexane	73.8	15.5 30.4 54.2
Acetic acid Benzene Cyclohexane	77.2	7.6 34.4 58.0	2-Propanol Benzene Cyclohexane	69.1	31.1 15.0 53.9
Acetic acid 2-Methyl-1-butanol Isopentyl acetate	132	15 54 31	1-Butanol Benzene Cyclohexane	77.4	4 48 48
Propionic acid 2-Methylpyridine Decane	149.3	29.5 32.0 38.5	1-Butanol Pyridine Toluene	108.7	11.9 20.7 76.4

Propionic acid 2-Methylpyridine Nonane	140.1	16.5 21.5 42.0	1,2-Ethanediol Phenol 2,6-Dimethylpyridine	185.0	8.7 74.6 16.7
Propionic acid 2-Methylpyridine Octane	123.7	4.5 10.5 85.0	1,2-Ethanediol Phenol 2-Methylpyridine	185.1	5.9 79.1 15.0
Propionic acid 2-Methylpyridine Undecane	153.4	43.0 40.0 17.0	1,2-Ethanediol Phenol 3-Methylpyridine	186.4	15.9 67.7 16.4
Propionic acid Pyridine Undecane	147.1	55.5 26.4 18.1	1,2-Ethanediol Phenol 2,4,6-Trimethylpyridine	188.6	29.5 54.8 15.7
Methanol Acetone Chloroform	57.5	23 30 47	Acetone Chloroform Hexane	60.8	3.6 68.8 27.6
Methanol Acetone Hexane	47	14.6 30.8 59.6	Acetone Methyl acetate Hexane	49.7	51.1 5.6 43.3
Methanol Acetone Methyl acetate	53.7	17.4 5.8 76.8	Chloroform Ethyl formate 2-Bromopropane	62.0	79.7 5.3 15.7
Methanol Methyl acetate Cyclohexane	50.8	17.8 48.6 33.6	1,4-Dioxane 2-Methyl-1-propanol Toluene	101.8	44.3 26.7 29.0

4.52 SECTION 4

FREEZING POINTS

Crystalline organic compounds typically have a characteristic melting point. In some cases, a compound may have more than one arrangement in the crystal and such polymorphs will exhibit differences in melting behavior. For the most part, however, the melting point of a compound is characteristic and invariant for a pure sample. When contaminated by a second substance, however, the melting (or freezing) point is typically lowered.

A classical test used to determine if two samples that have the same melting point are identical is to intimately mix them and record the melting point of the mixture. If the melting point of the blend is identical to that of each individual compound prior to mixing, the two substances are judged to be identical. When the two compounds are not the same, the melting point of the mixture is typically lowered and broadened.

The melting or freezing point depression can be used to determine an approximate molecular weight for a given substance. The cryoscopic constant K_f gives the depression of the melting point ΔT (in degrees Celsius) produced when 1 mol of solute is dissolved in 1000 g of a solvent. It is applicable only to dilute solutions for which the number of moles of solute is negligible in comparison with the number of moles of solvent. Because camphor is conveniently available and has a large K_f value, it is often used in this application. A known amount of the substance whose molecular weight is to be determined (the solute) is mixed with a larger amount of camphor (the solvent). Melting the mixture permits intimate mixing. The lowering or depression of the freezing point is then used to calculate the molecular weight from the following equation

$$M_2 = \frac{1000w_2K_f}{w_1\Delta T}$$

where M_2 is the molecular weight to be determined of the solute, w_1 is the exact weight of the solvent, w_2 is the exact weight of the added compound of unknown molecular mass, ΔT is the change in temperature, and K_f is the cryoscopic constant given in the Table 4.9A.

In Table 4.9A, a range of compounds and their cryoscopic constants are recorded. All of the same data are included in Table 4.9B but they are rearranged in order of increasing melting point at the left and decreasing K_t at the right.

TABLE 4.9A	Molecular Lowerin	g of the Melting	of Freezing Point
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Compound	K_f	MP	Compound	K_f	MP
Acetamide	4.04	80.1	Camphene	31.08	51–52
Acetic acid	3.90	16.63	Camphorquinone	45.7	199
Acetone	2.40	-95.35	D-(+)-Camphor	39.7	178.8
Ammonia	0.957	-77.75	Carbon tetrachloride	29.8	-22.9
Aniline	5.87	-5.98	o-Cresol	5.60	30.9
Antimony(III) chloride	17.95	73.4	p-Cresol	6.96	34.8
Benzene Benzonitrile Benzophenone Bicyclohexane	5.12 5.34 9.8 14.52	5.53 -12.75 48.1 3-4	Cyclohexane Cyclohexanol Cyclohexylcyclohexane Cyclopentadecanone	20.0 39.3 14.52 21.3	6.5 25.2 3–4 64–66
Biphenyl	8.0	68.8	Z-Decahydronaphthalene	19.47	-43.0
Borneol	35.8	204	<i>E</i> -Decahydronaphthalene	20.81	-30.4
Bornylamine	40.6	163	Dibenz[de,kl)anthracene	25.7	273-274
Butanedinitrile	18.26	57.9	Dibenzyl ether	6.27	3.5

TABLE 4.9A Molecular Lowering of the Melting of Freezing Point (*continued*)

Compound	K_f	MP	Compound	K_f	MP
1,2-Dibromoethane	12.5	10.0	Nitrobenzene	6.852	5.8
Diethyl ether	1.79	-116.3	Octadecanoic acid	4.50	70
1,2-Dimethoxybenzene	6.38	22.5	2-Oxohexa-		
N, N-Dimethylacetamide	4.46	-20.0	methyleneimine	7.30	69.2
2,2-Dimethyl-1-propanol	11.0	52–54	Phenol	7.40	40.9
Dimethyl sulfoxide	4.07	18.5	Pyridine	4.75	-41.6
1,4-Dioxane	4.63	11.7	*		
Diphenylamine	8.60	53–54	Quinoline	1.95	-14.9
Diphenyl ether	7.88	26.9	Succinonitrile	18.26	46-48
1,2-Ethanediamine	2.43	8.5	Sulfuric acid	1.86	10.38
Ethoxybenzene	7.15	-29.5	1,1,2,2,-Tetrabro-		
Formamide	3.85	2.6	moethane	21.7	0.0
Formic acid	2.77	8.5	1,1,2,2,-Tetrachloro1,2-	37.7	26.0
Glycerol	3.3-3.7	18.18	difluoroethane		
•			Tetramethylene sulfone	64.1	27.6
Hexamethylphos- phoramide	6.93	7.2	<i>p</i> -Toluidine	5.372	43.8
N-Methylacetamide	6.65	30.6	Tribromomethane	14.4	8.1
2-Methyl-2-butanol	10.4	-9.0	1,3,3-Trimethyl-2-	6.7	1–2
Methylcyclohexane	14.13	-9.0 -126.6	oxabicyclo[2.2.2]octane		
Methyl Z-9-octadecenoate	3.4	19.9	Triphenylmethane	12.45	93.4
2-Methyl -2-propanol	8.37	25.8	Water	1.86	0.000
Naphthalene Naphthalene	6.94	80.2	<i>p</i> -Xylene	4.3	13.3

The same data are presented in Table 4.9B but the information is rearranged at the left in order of increasing melting point and at the right in order of decreasing K_f .

TABLE 4.9B Molecular Lowering of the Melting of Freezing Point

Compound	K_f	MP	Compound	K_f	MP
Methylcyclohexane	14.13	-126.6	Tetramethylene sulfone	64.1	27.6
Diethyl ether	1.79	-116.3	Camphorquinone	45.7	199
Acetone	2.4	-95.35	Bornylamine	40.6	163
Ammonia	0.957	-77.75	D-(+)-Camphor	39.7	178.8
Z-Decahydronaphthalene	19.47	-43	Cyclohexanol	39.3	25.2
Pyridine	4.75	-41.6	1,1,2,2-Tetrachloro-1,2-	37.7	26
<i>E</i> -Decahydronaphthalene	20.81	-30.4	difluoroethane		
Ethoxybenzene	7.15	-29.5	Borneol	35.8	204
Carbon tetrachloride	29.8	-22.9	Camphene	31.08	51-52
N, N- Dimethylacetamide	4.46	-20	Carbon tetrachloride	29.8	-22.9
Quinoline	1.95	-14.9	Dibenz[de,kl)anthracene	25.7	273-274
Benzonitrile	5.34	-12.75	1,1,2,2-Tetrabromoethane	21.7	0
2-Methyl-2-butanol	10.4	-9	Cyclopentadecanone	21.3	64-66
Aniline	5.87	-5.98	E- Decahydronaphthalene	20.81	-30.4
1,1,2,2-Tetrabromoethane	21.7	0	Cyclohexane	20	6.5
Water	1.86	0	Z-Decahydronaphthalene	19.47	-43
1,3,3-Trimethyl-2-	6.7	1–2	Succinonitrile	18.26	46-48
oxabicyclo[2.2.2]octane			Butanedinitrile	18.26	57.9

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TABLE 4.9B Molecular Lowering of the Melting of Freezing Point (*continued*)

Compound	K_f	MP	Compound	K_f	MP
Formamide	3.85	2.6	Antimony(III) chloride	17.95	73.4
Bicyclohexane	14.52	3–4	Bicyclohexane	14.52	3–4
Dibenzyl ether	6.27	3.5	Cyclohexylcyclohexane	14.52	6.5
Benzene	5.12	5.53	Tribromomethane	14.4	8.1
Nitrobenzene	6.852	5.8	Methylcyclohexane	14.13	-126.6
Cyclohexane	20	6.5	1,2-Dibromoethane	12.5	10
Cyclohexylcyclohexane	14.52	6.5	Triphenylmethane	12.45	93.4
Hexamethyl-	17.52	0.5	Triplieny iniculanc	12.73	73.4
phosphoramide	6.93	7.2	2,2-Dimethyl-1-propanol	11	52-54
Tribromomethane	14.4	8.1	2-Methyl-2-butanol	10.4	-9
1.2-Ethanediamine	2.43	8.5	Benzophenone	9.8	48.1
Formic acid	2.77	8.5	Diphenylamine	8.6	53–54
1,2-Dibromoethane	12.5	10		8.37	25.8
*		10.38	2-Methyl-2-propanol		
Sulfuric acid	1.86		Biphenyl	8	68.8
1,4-Dioxane	4.63	11.7	Diphenyl ether	7.88	26.9
<i>p</i> -Xylene	4.3	13.3	Phenol	7.4	40.9
Acetic acid	3.9	16.63	2-Oxohexamethylene imine	7.3	69.2
Glycerol	3.3–3.7	18.18	Ethoxybenzene	7.15	-29.5
Dimethyl sulfoxide	4.07	18.5	p-Cresol	6.96	34.8
Methyl Z-9-octadecenoate	3.4	19.9	Naphthalene	6.94	80.2
1,2-Dimethoxybenzene	6.38	22.5	Hexamethylphosphoramide	6.93	7.2
Cyclohexanol	39.3	25.2	Nitrobenzene	6.852	5.8
2-Methyl-2-propanol	8.37	25.8	1,3,3-Trimethyl-2-		
1,1,2,2-Tetrachloro-1,2-	37.7	26	oxabicyclo[2.2.2]octane	6.7	1-2
difluoroethane			N-Methylacetamide	6.65	30.6
Diphenyl ether	7.88	26.9	1,2-Dimethoxybenzene	6.38	22.5
Tetramethylene sulfone	64.1	27.6	Dibenzyl ether	6.27	3.5
N-Methylacetamide	6.65	30.6	Aniline	5.87	-5.98
o-Cresol	5.6	30.9	o-Cresol	5.6	30.9
p-Cresol	6.96	34.8	p-Toluidine	5.372	43.8
Phenol	7.4	40.9	Benzonitrile	5.34	-12.75
p-Toluidine	5.372	43.8	Benzene	5.12	5.53
Succinonitrile	18.26	46–48	Pyridine	4.75	-41.6
Benzophenone	9.8	48.1	1,4-Dioxane	4.63	11.7
Camphene	31.08	51-52	Octadecanoic acid	4.5	70
2,2-Dimethyl-1-propanol	11	52–54	N, N- Dimethylacetamide	4.46	-20
Diphenylamine	8.6	53–54	<i>p</i> -Xylene	4.3	13.3
Butanedinitrile	18.26	57.9	Dimethyl sulfoxide	4.07	18.5
Cyclopentadecanone	21.3	64–66	Acetamide	4.04	80.1
Biphenyl	8	68.8	Acetic acid	3.9	16.63
2-Oxohexamethylene imine		69.2	Formamide	3.85	2.6
Octadecanoic acid	4.5	70	Glycerol	3.3–3.7	18.18
Antimony(III) chloride	17.95	73.4	Methyl Z-9-octadecenoate	3.4	19.9
Acetamide Acetamide	4.04	80.1	Formic acid	2.77	8.5
Naphthalene	6.94	80.1	1,2-Ethanediamine	2.43	8.5
1			· · · · · · · · · · · · · · · · · · ·	2.43	
Triphenylmethane	12.45	93.4	Acetone		-95.35
Bornylamine	40.6	163	Quinoline	1.95	-14.9
D-(+)-Camphor	39.7	178.8	Water	1.86	0
Camphorquinone	45.7	199	Sulfuric acid	1.86	10.38
Borneol	35.8	204	Diethyl ether	1.79	-116.3
Dibenz[de,kl) anthracene	25.7	273–274	Ammonia	0.957	-77.75

VISCOSITY, DIELECTRIC CONSTANT, DIPOLE MOMENT, SURFACE TENSION. AND REFRACTIVE INDEX

Several additional physical properties are summarized in Table 4.10. These are viscosity, dielectric constant, dipole moment, and surface tension for selected common organic compounds.

Viscosity

Viscosity may be thought of as a fluid's resistance to flow or internal friction. It is characterized by the property called viscosity, which is designated η (eta). A fluid passing through a tube will flow more freely if its viscosity is low and more slowly if it is more viscous. Viscosity is given in Table 4.10 in units of milliNewton·second·meter⁻² or mN·s·m⁻². In fluid mechanics, the unit "poise" is equal to a force of 1 dyne·cm⁻² for two fluids passing each other at a rate of 1 cm·s⁻¹. Viscosity is typically greater at lower temperatures; temperatures (in °C) are given in parentheses in the table.

Dielectric Constant

The dielectric constant (or relative permittivity) is usually expressed using the symbol ε . The dielectric ε is defined as the ratio of electric fields E_0/E for a vacuum and a substance placed between the plates of a capacitor. The dielectric constant of a vacuum is 1 and substances that can orient to greater or lesser extents in the applied field will have higher dielectric constants. The dielectric constant of heptane at 20°C is ~ 1.9 . Acetonitrile, $\text{CH}_3\text{C} \equiv \text{N}$:, has a dielectric constant at 20°C of 37.5. The dielectric constant for water is near 80.

The choice of a solvent for a particular reaction will usually depend on more than one variable. These include the liquid temperature range, the dielectric constant, and whether or not the solvent is reactive in the chemical reaction. The most important consideration in the latter context is often the presence of an easily transferred proton. Certain solvents, such as acetone, are considered aprotic but may transfer a proton under basic conditions. Thus the designations given below are general and approximate. They are intended to guide the reader to the more detailed information contained in the full tables.

Common Solvents Listed in Order of Increasing Dielectric Constant (Ascending Polarity)

Aprotio	Protic Solvents	
Dielectric constants < 15	Dielectric constants > 15	Dielectric range 6–80
carbon disulfide	acetone	acetic acid
carbon tetrachloride	benzonitrile	trifluoroacetic acid
tetrachloroethylene	hexamethylphosphoramide	phenols
1,2-dichloroethylene	<i>N</i> -methylpyrrolidone	butanols
chlorobenzene	nitrobenzene	propanols
dichloromethane	nitromethane	ethanol
chloroform	N,N-dimethylformamide (DMF)	2,2,2-trifluoroethanol
1,4-dioxane	acetonitrile	methanol
diphenyl ether	dimethyl sulfoxide (DMSO)	various glycols
diethyl ether	•	water

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Aprotic	Protic Solvents	
Dielectric constants < 15	Dielectric constants > 15	Dielectric range 6–80

tetrahydrofuran (THF) 1,2-dimethoxyethane (DME) ethyl acetate butyl acetate *N*,*N*-dimethylaniline pyridine

Dipole Moment

The dipole moment of a molecule is the vectorial sum of the individual dipoles within it. Bond dipoles are usually represented using the symbol μ and are expressed in units of Debye. The dipoles result from charge separation. The carbon–carbon bond in ethane, H_3C — CH_3 is symmetrical and not expected to have a dipole moment. The carbon–oxygen bond of methanol (CH_3OH), on the other hand, links two elements of differing electronegativity and is expected to have a significant molecular dipole. Methanol's molecular dipole is ~ 1.7 whereas, for ethane, it is 0.

Experimentally, the molecular dipole can be measured. Individual bond dipoles cannot be measured but they have been inferred from experimental data for a variety of compounds. Estimates of the molecular dipole can be made by vector addition of individual moments. Such estimates (calculations) are indicative but may differ significantly from the measured values. The latter are recorded in Table 4.10.

Four examples of dipole moments are instructive. First, the dipoles for chloromethane and dichloromethane are 1.87D and 1.60D, respectively. Although two chlorine–carbon bonds are present in the latter, the dipole is not along either but rather bisects the angle between them. This is illustrated schematically using the stylized arrow with its positive end in the form of a cross. The orientation question is shown clearly in the rigid dichlorobenzene framework. The dipole is 2.13D for the *ortho*-isomer and 0D when the dipoles exactly oppose each other.

The orientation of dipoles can be assessed by comparing otherwise identical molecules. For example, amino is electron releasing and nitro is electron withdrawing. The molecular dipoles $(1.53\,\mathrm{D}$ for aniline and $4.22\,\mathrm{D}$ for nitrobenzene) add to give an overall molecular dipole of $6.3\,\mathrm{D}$ for 4-nitroaniline. The importance of two polar C—O bonds should be large

if they are added and small if they oppose. The dynamics of the system must be taken into account for structures such as 1,2-dihydroxyethane (ethylene glycol), which is illustrated in the eclipsed and staggered conformers.

Surface Tension

The surface tension is the force that acts on the surface of a liquid that tends to minimize the surface area of the liquid. Surface tension is also sometimes referred to as interfacial force or interfacial tension. The property of surface tension is temperature dependent. For the majority of compounds the dependence of the surface tension γ on the temperature can be given as

$$\gamma = a - bt$$

where a and b are constants and t is the temperature in $^{\circ}$ C.

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances

States:	[g], gas	Solvents:	[B], benzene,	C_6H_6
	[lq], liquid		[C], carbon tetrachloride,	CCl_4
			[D], 1,4-dioxane,	$C_4H_8O_2$
			[H], hexane,	C_6H_{14}
			[cH], cyclohexane,	C_6H_{12}

The temperature in degrees Celsius at which the viscosity, dielectric constant, dipole moment, and surface tension of a substance were measured is shown in this table in parentheses after the value. The solvent used or the physical state of the substance are also shown in parentheses after the temperature in square brackets, for example, [g] or [b]

Alternate names for entries are listed in Table 1-14 at the bottom of each double page.

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant ε	Dipole moment, D	а	b
Acetaldehyde	0.280 (0) 0.256 (10) 0.22 (20)	21.8(10) 21.1 (21)	2.71 [g]	23.90	0.1360
Acetaldoxime	1.415 (20)	3 (23)	0.830 (20) [lq] 0.90 (25) [B]	30.1 (35)	
Acetamide	1.32 (105) 1.06 (120)	59.2 (83) 60.6 (94)	3 90 (25) [B] 2.44 (30) [B]	47.66	0.102 1
Acetanilide	2.22 (120) 1.90 (130)	3.65 (25) [B]	46.21	0.091 2	
Acetic acid	1.232 (20) 0.796 (50)	6.15 (20) 6.29 (40)	1 76[g] 1.92 (20) [B]	29.58	0.0094

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to dyn·ci	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Acetic anhydride	0.907 (20) 0.699 (40)	23.3 (0) 21.2 (20)	2.8 [g] 3.15 (20) [B]	35.52	0.143 6
Acetone [lq]	0.391 (0)	20.7 (25)	2.77 (22) [B]	26.26	0.112
[g]	0.318 (20) 0.009 33 (100) 0.012 8 (225)	17.6 (56) 1.015 9 (100)	2.87		
Acetonitrile	0.397 (10) 0.329 (30)	37.5 (20) 26.6 (82)	3.97 [g] 3.47 (20) [B]	29.58	0.1178
Acetophenone	2.015 (15) 1.511 (30)	17.39 (25) 8.64 (202)	2.96 (30) [B]	41.92	0.1154
Acetyl bromide Acetyl chloride		16.2 (20)	2.45 (20) [B]		
[lq]		16.9 (2) 15.8 (22)	2.47 (20) [B]	26.7 (15)	
[g] Acetylene [g]	0.010 2 (30) 0.012 6 (101)	1.0217 (20) 1.001 34 (0)	2.71	3.42	0.193 5 [lq]
Acrylic acid	1.3 (20) 1.16 (25)			28.1 (30)	
Acrylonitrile	0.35 (20) 0.34 (25)	33.0 (20)	3.91 [g] 3.54 (25) [B]	29.58	0.1178
Allylamine	0.207 (30) 0.375 (25)		1.3 (25) [B]	28.73 27.49	0.118 6 0.128 7
Allyl isothiocyanate	0.070 (20)	17.2 (18)	3.2 (20) [B]	36.76	0.107 4
2-Aminoethanol	30.85 (15) 19.35 (25)	37.72 (25)	2.59 (25) [D]	51.11	0.1117
Aniline	5.30 (15) 4.40 (20) 3.18 (30)	6.89 (20) 5.93 (70)	1.53 (20) [B]	44.83	0.108 5
Benzaldehyde	1.321 (25)	19.7 (0) 17.8 (20)	2.77 (20) [lq]	40.72	0.1090
Benzaldehyde oxime (mp 30)		3.8 (20)	1.2 (25) [B]		
(mp 128) Benzene	0.649 (20) 0.566 (30)	2.292 (15) 2.274 (25)	1.5 (25) [B] 0	28.88 (20)	27.56 (30)
Benzamide Benzenesulfonyl chloride	0.395 (60)	1.002 8 [g]	3.42 (25) [B] 4.50 (20) [B]	47.26 45.48	0.070 5 0.111 7
Benzenethiol	1.239 (20) 1.144 (25)	4.38 (25)	1.13 (25) [lq] 1.19 (20) [B]	41.41	0.1202

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Benzonitrile	1.447 (15) 1.111 (30)	26.5 (20) 24.0 (40)	4.40 [g] 3.9 (20) [B]	41.69	0.1159
Benzophenone	4.79 (55) 1.38 (120)	14.60 (18) 11.4 (50)	3.09 (50) [lq] 2.98 (25) [B]	46.31	0.1128
Benzoyl bromide	1.956 (20) 1.798 (25)	21.33 (20) 20.74 (25)	3.40 (20) [B]	45.85	0.1397
Benzoyl chloride		29 (0) 23 (20)	3.16 (25) [B]	41.34	0.108 4
Benzyl acetate Benzyl alcohol	1.399 (45) 5.58 (20) 4.65 (30) 3.01 (45)	5.1 (21) 13.0 (20) 9.5 (70)	1.80 (25) [B] 1.67 (25) [B]	38.25	0.138 1
Benzylamine	1.59 (25)	5.5 (1) 4.6 (21)	1.15 (20) [lq] 1.38 (25) [B]	42.33	0.1213
Benzyl benzoate Benzyl butyl	8.51 (25)	4.9 (20)	2.06 (30) [B]	48.07	0.106 5
o-phthalate Benzyl chloride	65 (20) 1.400 (20) 1.290 (25)	7.0 (13)	1.83 (20) [B]	39.92	0.1227
Benzylethylamine Benzyl ethyl ether Biphenyl Bis(2-ethoxyeth-	, ,	4.3 (20) 3.9 (20) 2.53 (75)	0 1.92 (25) [B]	32.83 (20) 41.52 29.74	29.97 (40) 0.093 1 0.117 6
yl)ether Bis(2-hydroxye- thyl)ether 1,2-Bis(methoxy- ethoxy)-ethane	38.0 (20) 30.0 (25) 3.76 (20)	31.69 (20)	2.31 (20) [B]	46.97	0.088 0
Bis(2-methoxy- ethyl) ether	1.99 (20)		1.97 (25) [B]	32.47	0.1164
DL-Bornyl acetate 3-Bromoaniline	0.981 (25) 6.81(20) 3.70 (40)	4.6 (21) 13.0 (19)	1.89 (22) 2.67 (20) [B]		
4-Bromoaniline Bromobenzene	1.81 (80) 1.196 (15) 0.985 (30)	7.06 (30) 5.40 (25)	2.88 (25) [B] 1.70 [g] 1.50 (20) [lq]	38.14	0.1160
1-Bromobutane	0.633 (20) 0.597 (25)	7.88 (-10) 7.07 (20)	2.17 [g] 2.04 (20) [lq]	28.71	0.1126
DL-2-Bromobutane	1.434 (20)	8.64 (25)	2.22 [g] 2.14 (25) [lq]	27.48	0.1107
1-Bromo-2- chlorobenzene 1-Bromo-3-		6.80 (20) 4.58 (20)	2.15 (20) [B] 1.52 (22) [B]		
chlorobenzene 1-Bromo-4- chlorobenzene		4.30 (20)	0.1 (25) [B]	40.03	0.100 2

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Bromochloro- methane	0.670 (20)	7.79	1.66 (25) [B]	33.32 (20)	
Bromocyclo-	2.0 (25)	11 (-65)	1.08 (25) [lq]	36.13	0.1117
hexane 1-Bromodecane		7.9 (25) 4.75 (1) 4.44 (25)	2.3 (25) [B] 2.08 (20) [lq] 1.90 (25) [lq]	31.26	0.085 6
Bromodichloro- methane		4.44 (23)	1.90 (23) [tq] 1.31 (25) [B]	35.11	0.1294
1-Bromododecane		4.07 (25)	2.01 (25) [lq] 1.89 (25) [B]	32.58	0.088 2
Bromoethane	0.397 (20) 0.348 (30)	13.6 (-60) 9.39 (20)	2.03 [g] 2.04 (20) [lq]	26.52	0.1159
1-Bromo-2- ethoxyethane)		31.98	0.1129
1-Bromo-2- ethoxypentane		6.45 (25)	2.32 (25) [B]		
2-Bromo-2- ethoxypentane		6.40 (25)	2.07 (25) [B]		
3-Bromo-3- ethoxypentane		8.24 (25)	2.15 (25) [B]		
Bromoethylene		4.78 (25)	1.42 [g]		
Bromoform	2.152 (15) 1.741 (30)	4.39 (20)	1.00 [g] 0.92 (25) [lq]	48.14	0.1308
1-Bromoheptane		5.33 (25) 4.48 (90)	2.17 [g] 2.02 (20) [lq]	30.74	0.098 2
2-Bromoheptane 3-Bromoheptane		6.46 (22) 6.93 (22)	2.08 (20) [B] 2.06 (20) [B]		
4-Bromoheptane		6.81 (22)	2.06 (20) [B]		
1-Bromohexa-		3.71 (25)	1.98 (20) [lq]	33.37	0.086 1
decane			1.96 (25) [C]		
1-Bromohexane		6.30 (1) 5.82 (25)	2.06 (20) [lq]	29.81	0.0967
Bromomethane		9.82 (0) 1.006 8 (100) [g]	1.79 [g]	26.52	0.1159
1-Bromo-3- methylbutane		8.04 (-56) 6.05 (20)	1.95 (20) [B]	28.10	0.0996
2-Bromo-3- methylbutyric acid		6.5 (20)			
1-Bromo-2- methylpropane	0.643 (20) 0.518 (40)	7.70 (0) 7.2 (25)	1.92 (25) [lq] 1.99 (20) [B]	26.96	0.105 9
1-Bromonaph-	3.26 (90) 5.99 (15)	5.83 (25)	1.29 (25) [lq]	46.44	0.101 8
thalene 1-Bromononane	3.20 (40)	5.12 (20) 5.42 (-20) 4.74 (25)	1.95 (25) [lq]	31.36	0.0894

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
1-Bromooctane		6.35 (-50)	1.99 (20) [lq] 1.88 (25) [lq]	31.00	0.0928
1-Bromopenta- decane		3.9 (20)	() t B		
1-Bromopentane		9.9 (-90) 6.32 (25)	2.21 [g] 2.09 (20) [lq]	29.51	0.1049
p-Bromophenol		0.32 (23)	2.09 (20) [iqj	48.88	0.1070
1-Bromopropane	0.539 (15) 0.459 (30)	8.09 (25)	2.17 [g] 3.16 (20) [lq]	28.30	0.1218
2-Bromopropane	0.536 (15) 0.437 (30)	9.46 (25)	2.21 [g] 2.10 (25) [lq]	26.21	0.1183
1-Bromotetra- decane		3.84 (25)	1.92 (20) [lq] 1.83 (25) [lq]	32.93	0.087 8
<i>o</i> -Bromotoluene <i>m</i> -Bromotoluene	1.3 (25)	4.28 (58) 5.36 (58)	1.45 (20) [B] 1.77 (20) [B]	36.62	0.0998
<i>p</i> -Bromotoluene		5.49 (58)	1.95 (20) [B]	36.40	0.0997
Bromotrifluoro- methane	0.15 (25)	()	0.65 [g]	4 (25)	
1-Bromoundecane	e	4.73(-9)		31.94	0.086 1
Butane	0.007 39 (20) [g]		0	14.87	0.1206
	0.008 39 (60) [g]				
1,3-Butanediol	130.3 (20) 89 (25)	28.8 (25)		37.8 (25)	
1,4-Butanediol	65–70 (25)	33 (15) 30 (30)	3.93 (20) [lq] 2.4 (15) [D]		
2,3-Butanediol	121 (25)		. , , , , ,	36 (25)	
Butanesulfonyl chloride			3.94 (25) [D]	37.33	0.0977
1-Butanethiol	0.501 (20) 0.450 (30)	5.07 (25) 4.59 (50)	1.54 (25) [lq] or [B]	28.07	0.1142
1,2,4-Butanetriol	1227 (25)				
1-Butanol	2.948 (20)	17.8 (20)	1.66 [g]	27.18	0.0898
	1.782 (40)	8.2 (118)	20 [B]		
DL-2-Butanol	3.907 (20) 0.527 (100)	16.6 (25)	1.66 (30) [B]	23.47 (20)	22.62 (30)
2-Butanone	0.428 (20) 0.349 (40)	18.5 (20) 15.3 (60)	3.2 (30) [lq] 2.76 (25) [B]	26.77	0.1122
2-Butanone oxime		3.4 (20)	2.70 (23) [B]	31.89	0.1022
1-Butene [g]	0.007 6 (20) 0.010 0 (120)	1.003 2 (20)	0.30	15.19	0.132 3[lq]
2-Butene	(120)		0.33 [g, cis] 0 [g, trans]	16.11	0.1289
3-Butenenitrile		28.1 (20)	4.53 [g]	31.40	0.108 5
2-Butoxyethanol	3.15 (25) 1.51 (60)	9.30 (25)	2.08 (25) [B]	28.18	0.081 6
Butoxyethyne		6.62 (25)	2.05 (25) [Iq]		

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
2-(2-Butoxyeth- oxy)ethanol	4.76 (25)			30.0 (25)	
1-Butoxy-2- propanol	2.55 (25)			26.5 (25)	
Butyl acetate	0.734 (20) 0.688 (25)	6.85 (-73) 5.01 (20)	1.86 (22) [B]	27.55	0.1068
DL-sec-Butyl acetate	0.000 (23)	3.01 (20)		23.33 (22)	21.24 (42)
tert-Butyl acetate			1.91 (25) [B]	24.69	0.1102
Butylamine	0.681 (20)	4.88 (20)	1.00 [g] 1.22 (20) [lq]	26.24	0.1122
sec-Butylamine		4.4 (21)	1.28 (25) [B]	23.75	0.105 7
tert-Butylamine		l ` ´	1.29 (25) [B]	19.44	0.1028
Butylbenzene	1.035 (20) 0.960 (25)	2.36 (20)	0.36 (20) [lq]	31.28	0.102 5
sec-Butylbenzene		2.36 (20)	0.37 (20) [lq]	30.48	0.0979
tert-Butylbenzene		2.37 (20)	0.36 (20) [lq]	30.10	0.098 5
Butyl butyrate	0.84(25)			27.65	0.096 5
Butyl decyl o-phthalate	55 (20)				
N-Butyldietha- nolamine	55 (25)				
4- <i>tert</i> -Butyl-2,5-dimethylphenol	8.30 (80)				
4- <i>tert</i> -Butyl-2,6-dimethylphenol	2.72 (80)				
6- <i>tert</i> -Butyl-2,4-dimethylphenol	2.10 (80)				
6- <i>tert</i> -butyl-3,4-dimethylphenol	3.50 (80)				
N-Butylethano- lamine	17.4 (25)				
Butyl ethyl ether	0.421 (20) 0.397 (25)		1.24	22.75	0.1049
Butyl formate	0.691 (20) 0.940 (0)	2.43 (80)	2.08 (26) [lq] 2.03 (25) [B]	27.08	0.1026
Butyl methyl ether	> .0 (0)		1.25 (25) [B]	22.17	0.105 7
2- <i>tert</i> -Butyl-4- methylphenol	2.55 (80)		1.31 (20) [B]		
Butyl nitrate		13 (20)	2.99 (20) [B]	30.35	0.1126
2-(2-sec-Butylph- enoxy)ethanol	65.1 (25)	15 (20)	2.55 (20) [B]	30.33	5.1120
2-(4-tert-Butylph-	122.5 (25)				
enoxy)ethanol Butyl propionate			1.79 (22) [B]	27.37	0.0993

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
4- <i>tert</i> -Butyl-pyridine	1.495 (20)		2.87 (25) [C]	35.48	0.095 1
Butyl stearate	8.26 (25) 4.9 (50)	3.11 (30)	1.88 (24) [B]	33.0 (25)	32.7 (30)
Butyl vinyl ether	0.5 (20)		1.25 (25) [H]	21.99 (20)	
Butyraldehyde	0.455 (20) 0.367 (39)	13.4 (26)	2.45 (40) [lq]	26.67	0.092 5
Butyric acid	1.540 (20) 0.980 (40)	2.97 (20)	1.65 (30) [B]	28.35	0.092 0
Butyric anhydride	1.615 (20) 1.486 (25)	13 (20)		28.93 (20)	28.44 (25)
4-Butyrolactone Butyronitrile	1.75 (25) 0.624 (15) 0.515 (30)	39.1 (20) 20.3 (21)	4.12 (25) [B] 4.07 [g] 3.6 (20) [B]	29.51	0.103 7
Camphor		11.35 (20)	2.91 (20) [B] 3.10 (25) [B]		
Carbon disulfide	0.363 (20)	3.0 (-112) 2.64 (20)	0 [g] 0.12 (20) [lq]	35.29	0.1484
Carbon tetra- chloride	0.965 (20) 0.793 (25)	2.24 (20) 2.23 (25)	0	29.49	0.1224
Carbon tetra- fluoride	0.020 (25)	1.000 6 (25) [g]	0	14 (-73)	
Carvone		11 (22)	2.8 (15) [B]	36.54	0.0920
Chloroacetic acid	3.15 (50) 1.92 (75)	20 (20) 12.3 (60)	2.31 (30) [B]	43.27	0.1117
o-Chloroanilinem-Chloroaniline	0.925 (25)	13.4 (25) 13.4 (19)	1.78 (20) [B] 2.68 (20) [B]	43.41	0.0904
<i>p</i> -Chloroaniline			2.99 (25) [B]	48.69	0.109 9
Chlorobenzene	0.799 (20)	5.71 (20)	1.72 [g]	35.97	0.119 1
1-Chlorobutane	0.631 (40) 0.469 (15)	4.2 (120) 9.07 (-30)	1.56 (20) [lq] 2.13 [g]	25.97	0.1117
2-Chlorobutane	0.439 (15)	7.39 (20) 7.09 (30)	2.0 (20) [B] 2.14 [g] 2.1 (20) [B]	24.40	0.1118
Chlorocy- clohexane		10.9 (-47) 7.6 (25)	2.2 (25) [B]	33.90	0.110 1
Chlorodifluoro- methane	0.23 (25) 0.013 (25) [g]	6.11 (24)	1.4 [g]	8 (25)	
1-Chlorododecane	0.015 (25) [g]	4.2 (20)	2.11 (25) [lq] 1.94 (20) [B]	31.56	0.0904
1-Chloro-2-2,3- epoxypropane	1.03 (25)	25.6 (1) 22.6 (22)	1.8 (25) [C]	39.76	0.1360
Chloroethane	0.279 (10)	1.013 (19) [g]	2.0 [g] 1.96 (20) [lq]	21.18 (5)	20.58 (10)
2-Chloroethanol	3.913 (15)	25.8 (25) 13 (132)	1.77 [g] 1.90 (25) [B]	38.9 (20)	

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Chloroform	0.596 (15) 0.514 (30)	4.81 (20) 4.31 (50)	1.1 [g] 1.1 (25) [lq]	29.91	0.129 5
1-Chloroheptane 2-Chloroheptane 3-Chloroheptane	0.511(50)	4.48 (20) 6.52 (22) 6.70 (22)	1.86 (22) [B] 2.05 (22) [B] 2.06 (22) [B]	28.94	0.096 1
4-Chloroheptane 1-Chlorohexane Chloromethane		6.54 (22)	2.06 (22) [B] 1.94 (20) [B]	28.32	0.103 8
[g]	0.0106 (20) 0.012 9 (80)	1.006 9 (100)	1.87		
[lq] 1-Chloro-3- methylbutane		12.6 (-20) 7.63 (-70) 6.05 (20)	1.86 (20) 1.94 (20) [B]	19.5 25.51	0.165 0 0.107 6
Chloromethyl methyl ether			1.88 [C]		
1-Chloro-2- methylpropane	0.462 (20) 0.373 (40)	7.87 (-38) 6.49 (14)	2.06 [g] 2.0 (25) [B]	24.40	0.1099
2-Chloro-2- methylpropane	0.543 (15)	10.95 (0) 9.96 (20)	2.11 [g] 2.13 (25) [B]	20.06 (15)	18.35 (30)
1-Chloronaph- thalene	2.940 (25)	5.04 (25)	1.33 (25) [lq] 1.52 (25) [B]	44.12	0.103 5
o-Chloronitro- benzene		38 (50) 32 (80)	4.62 [g] 6.22 (50) [lq]	48.10	0.117 1
<i>m</i> -Chloronitro- benzene		21 (50) 18 (80)	3.72 [g] 3.30 (50) [lq]	49.71	0.1417
<i>p</i> -Chloronitrobenzene		8 (120)	2.81 [g] 2.83 (90) [lq]	45.84	0.1046
1-Chlorooctane Chloropenta- fluoroethane	0.26 (25) 0.013 (25) [g]	5.05 (25)	2.14 (25) [lq] 0.5 [g]	29 64 5 (25)	0.096 1
1-Chloropentane	0.580 (20)	6.6 (11)	2.14 [g] 1.94 (20) [B]	27.09	0.1076
o-Chlorophenol	2.250 (45) 4.11 (25)	6.31 (25)	2.19 [g] 1.46 (20) [lq]	42.5	0.1122
m-Chlorophenol	4.722 (45) 11.55 (25)		2.19 (25) [B]	43.7	0.1009
<i>p</i> -Chlorophenol 1-Chloropropane	4.99 (50) 0.372 (15)	7.7 (20)	2.09 (20) [B] 2.05 [g]	19.51 24.41	0.087 5 0.124 6
2-Chloropropane	0.318 (30) 0.335 (15) 0.299 (30)	9.82 (20)	1.96 (20) [B] 2.17 [g] 2.1 (20) [B]	21.37	0.0883
1-Chloro-2- propanone		30 (19)	2.22 [g] 2.37 (20), [H]		
3-Chloro-1- propene	0.347 (15)	8.2 (20)	2.0 [g] 1.8 (20) [B]	25.50	0.0946

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface t	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
o-Chlorotoluene		4.45 (20)	1.57 [g]		
<i>m</i> -Chlorotoluene		4.2 (55) 5.5 (20) 5.0 (60)	1.41 (20) [lq] 1.77 (20) [lq]		
p-Chlorotoluene		6.08 (20) 5.6 (55)	1.8 (22) [B] 2.21 [g] 1.90 (20) [lq]	34.93	0.108 2
Chlorotrifluoro- methane	0.016 (25)	1.001 3 (29) [g]	0.50 [g]	14 (-73)	
Chlorotrimethy- lsilane			2.09 (20) [B]	19.51	0.087 5
Cinnamaldehyde		17 (20)	3.74 [g]		
. C1	2.506 (46)	16.9 (24)	3.30 (30) [lq]	20.42	0.101.1
o-Cresol	3.506 (46)	11.5 (25)	2.32 (25) [lq] 1.45 (25) [B]	39.43	0.101 1
m-Cresol	18.42 (20)	11.8 (25)	2.39 (20) [lq]	38.00	0.0924
m cresor	5.057 (45)	11.0 (23)	1.61 (25) [B]	30.00	0.072
p-Cresol	5.607 (45)	9.91 (58)	2.35 (20) [lq]	38.58	0.0962
•			1.54 (20) [B]		
Crotonic acid			2.13 (30) [B]		
Cyanoacetic acid		33.4 (19)			
Cycloheptanol 1,3-Cyclohex- adiene		2.6 (-89)	0.38 (20) [B]	35.02	0.0923
Cyclohexane	0.980 (20) 0.534 (60)	2.05 (15) 2.02 (25)	0	27.62	0.1188
Cyclohexane- carboxylic acid		2.6 (31)			
1,4-Cyclohex- anedione		15.0 (25)	1.41 [g] 1.3 (30) [B]		
Cyclohexanol	41.07 (30) 17.19 (45)	15.0 (25) 7.24 (100)	1.86 (25) [C]	35.33	0.0966
Cyclohexanone	2.453 (15)	20 (-40)	3.11 (20) [B]	37.67	0.1242
Cyclohexanone	1.803 (30)	18.2 (20) 3.0 (89)	3.01 (25) [B] 0.83 (25) [B]		
oxime Cyclohexene	0.650 (20)	2.6 (-105)	0.61 [g]	29.23	0.122 3
c) elonement	0.050 (20)	2.22 (25)	0.28 (20) [lq]	25.25	0.1223
Cyclohexylamine	1.662 (20) 1.16 (49)	4.73 (20)	1.22 (20) [lq] 1.26 (20) [B]	34.19	0.1188
Cyclohexyl-	3.681 (0)		0.62 (20) [B]		
benzene					
Cyclohexyl-		9.7 (60)	1.68 (20) [B]		
methanol		8.1 (80)			
o-Cyclohexyl- phenol		3.97 (55)			

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance mN·s·m ⁻² constant, ε moment, D a b p-Cyclohexyl-phenol 4.42 (131) 32.02 0.109 0 Cyclopentane 0.439 (20) 1.965 (20) 0 25.53 0.146 2 Cyclopentanol 25 (-20) 1 72 (25) [C] 35.04 0.101 1 Cyclopentanone 16 (-51) 3.30 [g] 35.55 0.110 0 Cyclopentene 2.93 (25) [B] 0.98 (25) [H] 25.94 0.149 5 Cyclopentene 0.087 7 0 [lq] 28.83 0.087 7 cis-Decahydronaphthalene 3.381 (20) 2.18 (20) 0 32.18 (20) 31.01 (30)					Surface to dyn·cr	
Denoil Cyclopentane Cyclopentene Cyclopentene Cyclopentene Cyclopentene Cyclopentene Cyclopentene Cyclopentane	Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Cyclopentane Cyclopentanol 0.439 (20) 1.965 (20) 25 (-20) 18 (20) 0 32.02 25.53 0.109 0 0.149 0 0.101 1 Cyclopentanone Cyclopentanone 0.439 (20) 1.965 (20) 25 (-20) 18 (20) 1.72 (25) [C] 35.04 3.100 0 0.101 1 Cyclopentanone P-Cymene P-Cymene P-Cymene Sis-Decahydro- naphthalene trans-Decahydro- naphthalene Decamethyley- clopentasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylte- trasiloxane Decamethylene Dibenzyl ether P-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene p-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene m-Dibromobenzene p-Dibromobenzene m-Dibrom			4.42 (131)			
Cyclopentane Cyclopentanol 0.439 (20) 1.965 (20) 25 (-20) 18 (20) 0 172 (25) [C] 25.53 35.04 0.146 2 0.101 1 Cyclopentanone Cyclopentene p-Cymene 3.402 (20) 2.243 (20) 0 [1] 2.93 (25) [B] 25.94 0.149 5 Cyclopentene p-Cymene 3.402 (20) 2.243 (20) 0 [1] 28.83 0.087 7 cis-Decahydro- naphthalene trans-Decahydro- naphthalene Decamethylte- trasiloxane Decamethylte- trasiloxane Decame 2.128 (20) 2.17 (20) 0 29.89 (20) 31.01 (30) 1-Decane 0.928 (20) 2.991 (20) 0.79 (25) [1q] 86.20 (25) 25.67 0.092 0 1-Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decane 0.805 (20) 1.33 (25) [B] 30.34 0.073 2 1-Decane 0.805 (20) 1.33 (25) [B] 30.34 0.073 2 1-Decane 0.305 (20) 1.33 (25) [B] 30.34 0.073 2 1-Decane 0.305 (20) 1.33 (25) [B] 30.42 (20)				0	32.02	0.109.0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		0.439 (20)	1.965 (20)	-		
Cyclopentanone 18 (20) 16 (-51) 3.30 [g] 2.93 (25) [B] 0.98 (25) [H] 25.94 0.110 0 Cyclopentene p-Cymene 3.402 (20) 2.243 (20) 0 [lq] 28.83 0.087 7 cis-Decachydronaphthalene trans-Decathydronaphthalene Decamethyleyclopentasiloxane Decamethyleycranional colored and potential decamethyle trasiloxane 2.128 (20) 2.17 (20) 0 29.89 (20) 28.87 (30) Decane 0.928 (20) 1.991 (20) 0 0.79 (25) [lq] 86.20 (25) 1-Decanol 1.28 (20) 2.4 (20) 0.79 (25) [lq] 86.20 (25) 0.092 0 1-Decanol 1.28 (20) 1.991 (20) 0 25.67 0.092 0 1-Decanol 8.1 (20) 1.71 (20) [B] 30.34 0.073 2 1-Decanol 8.1 (20) 1.71 (20) [B] 30.34 0.073 2 1-Decane 0.805 (20) 4.9 (20) 1.33 (25) [B] 0.94 (20) [B] 25.84 0.091 9 Dibenzyl decanedioate Dibenzyl decanedioate Dibenzyl ether o-Dibromobenzene p-Dibromobenzene p-Dibromoben		01.157 (20)				
Cyclopentene p-Cymene 3.402 (20) 2.243 (20) 0 [lq] 25.94 0.149 5 0.087 25 [H] 0.98 (25) [H] 0.98 (25) [H] 0.087 3 0.087 7 0.087 3 0.092 0 22.887 (30) 0.056 5 0.075 (25) [B] 0.073 (25) [B] 0.073 (25) [B] 0.073 (25) [B] 0.073 (7 1			. , , ,		
p-Cymene 3.402 (20) 2.243 (20) 0 [lq] 28.83 0.0877 cis-Decahydronaphthalene trans-Decahydronaphthalene trans-Decahydronaphthalene Decamethylcy-clopentasiloxane Decamethylcy-clopentasiloxane Decamethylcy-clopentasiloxane Decane 2.128 (20) 2.17 (20) 0 29.89 (20) 28.87 (30) Decamethylcy-clopentasiloxane Decamethylter trasiloxane 0.928 (20) 1.991 (20) 0 7.97 (25) [lq] 86.20 (25) 1-Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decanel 0.805 (20) 1.844 (130) 1.71 (20) [B] 30.34 0.073 2 1-Decene 0.805 (20) 1.844 (130) 1.71 (20) [B] 30.34 0.073 2 1-Decene 0.805 (20) 4.9 (20) 1.33 (25) [B] 30.34 0.073 2 1-Decene 0.805 (20) 1.33 (20) 1.33 (25) [B] 30.90 (20) [B] 43.27 0.108 6 Dibenzyl decanedioate Dibenzyl ether o-Dibromobenzene m-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobenzene (1,4-Dibromobutane p-Dibromobenzene (1,4-Dibromobutane p-Dibromobenzene (1,4-Dibromobutane (1,4-Dibromobutane p-Dibromobenzene (1,4-Dibromobutane (1,2-Dibromobutane (1,2-Dibromobutane (1,2-Dibromobutane (1,2-Dibromobutane (1,2-Dibromobutane	Cyclopentanone		16 (-51)		35.55	0.1100
cis-Decahydronaphthalene trans-Decahydronaphthalene trans-Decahydronaphthalene trans-Decahydronaphthalene Decamethylcy-clopentasiloxane Decamethyltetrasiloxane Decame (1.28 (20)) 2.18 (20) 2.17 (20) 0 29.89 (20) 28.87 (30) Decamethylcy-clopentasiloxane Decame Evans-Decane (1.28 (20)) 1.28 (20) 2.4 (20) 0.79 (25) [lq] 86.20 (25) Decane (1.28 (20)) 1.991 (20) 0 25.67 0.092 0 1-Decane (1.28 (20)) 1.991 (20) 0 25.67 0.092 0 1-Decane (1.28 (20)) 1.844 (130) 1.71 (20) [B] 30.34 0.073 2 1-Decene (1.28 (20)) 1.844 (130) 1.71 (20) [B] 30.34 0.073 2 1-Decene (1.28 (20)) 0.805 (20) 1.33 (25) [B] 0.42 (20) [B] 25.84 0.091 9 1-Decene (1.28 (20)) 0.805 (20) 1.33 (25) [B] 0.97 (20) [lq] 43.27 0.108 6 Dibenzyl decanedioate (1.28 (20)) 3.711 (25) 1.39 (21) [B] 38.2 (35) 38.2 (35) Dibenzyl ether (1.4-Dibromobenzene (1.4-Di	Cyclopentene			0.98 (25) [H]	25.94	0.149 5
naphthalene trans-Decahydronaphthalene 2.128 (20) 2.17 (20) 0 29.89 (20) 28.87 (30) Decamethylcyclopentasiloxane 2.5 (20) 19.56 0.056 5 Decamethyltetrasiloxane 0.28 (20) 2.4 (20) 0.79 (25) [lq] 86.20 (25) Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decane 0.805 (20) 1.844 (130) 1.71 (20) [B] 30.34 0.073 2 1-Decene 0.805 (20) 1.34 (20) 1.71 (20) [B] 30.34 0.073 2 1-Decene 0.805 (20) 1.33 (25) [B] 25.84 0.091 9 Dibenzyl decanedioate 3.0 (100) 0.88 (25) [B] 25.84 0.091 9 Dibenzyl decanedioate 3.6 (20) 0.97 (20) [Iq] 43.27 0.108 6 Dibenzyl ether o-Dibromobenzene m-Dibromobenzene m-Dibromobenzene p-Dibromobenzene 1,4-Dibromobutane 3.80 (20) 1.5 (20) [B] 38.2 (35) 2,3-Dibromobutane 5.75 (25) 2.20 [g] 1.7 (25) [Iq] 48.24 0.119 0 2,2-Dibromoethylene trans-1,2-Dibromoethylene romoethylene 1,2-Dibromoethylene 1,2-Dibromoeth	<i>p</i> -Cymene	3.402 (20)	2.243 (20)	0 [lq]	28.83	0.0877
trans-Decahydronaphthalene 2.128 (20) 2.17 (20) 0 29.89 (20) 28.87 (30) Decamethylevolopentasiloxane 1.28 (20) 2.4 (20) 0.79 (25) [lq] 86.20 (25) Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decane 0.928 (20) 1.991 (20) 0 25.67 0.092 0 1-Decanol 8.1 (20) 1.71 (20) [B] 30.34 0.073 2 1-Decane 0.805 (20) 1.34 (20) 1.33 (25) [B] 25.84 0.091 9 Diblenzofuran 3.0 (100) 0.88 (25) [B] 25.84 0.091 9 Dibenzyl decanedioate Dibenzyl ether o-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobutane 7.35 (20) 1.39 (21) [B] 38.2 (35) 2,3-Dibromobutane 5.75 (25) 2.20 [g] 48.24 0.119 0 2,3-Dibromobutane 1.721 (20) 4.78 (25) 1.11 [g] 35.43 0.142 8 2,2-Dibromoethylene trans-1,2-Dibromoethylene trans-1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibro	•	3.381 (20)	2.18 (20)	0	32.18 (20)	31.01 (30)
Decamethyley-clopentasiloxane Decamethylte-trasiloxane Decamethylte-trasiloxane Decamethylte-trasiloxane Decame Decam	trans-Decahydro-	2.128 (20)	2.17 (20)	0	29.89 (20)	28.87 (30)
Decamethyltetrasiloxane Decane De	Decamethylcy-		2.5 (20)		19.56	0.056 5
Decane		1.28 (20)	2.4 (20)	0.79 (25) [lq]	86.20 (25)	
1-Decanol 1-Decene 1-Decene 1-Decene 1-Decene 0.805 (20) 0.808 (25) [B] 0.42 (20) [B] 0.808 (25) [B] 0.97 (20) [Iq] 1.02 (20) [B] 0.97 (20) [Iq] 1.02 (20) [B] 0.97 (20) [Iq] 1.02 (20) [B] 0.100 (20) [B] 0.1	•	, ,		\ \ / L 13	` ′	
1-Decene	Decane	0.928 (20)	1.991 (20)	0	25.67	0.0920
1-Decene		0.775 (22)	1.844 (130)			
Diallyl sulfide Dibenzofuran Dibenzylamine	1-Decanol		8.1 (20)	, , ,	30.34	0.073 2
Dibenzofuran Dibenzylamine 3.0 (100) 0.88 (25) [B] 0.97 (20) [lq] 43.27 0.108 6	1-Decene	0.805 (20)		0.42 (20) [B]	25.84	0.0919
Dibenzylamine 3.6 (20) 0.97 (20) [lq] 1.02 (20) [B] 43.27 0.108 6			1 1			
Dibenzyl decanedioate Dibenzyl ether o-Dibromobenzene m-Dibromobenzene p-Dibromobenzene p-Dibromobenzene 1,4-Dibromobutane 2,3-Dibromobutane 1.721 (20) 4.78 (25) 4.6 (25) 1.39 (21) [B] 38.2 (35) 2.13 (20) [B] 38.2 (35) 2.15 (20) 2.13 (20) [B] 41.84 2.15 (20) [B] 41.84 2.16 (20) [B] 42.06 (20) [B] 42.06 (20) [B] 48.24 2.17 (25) [B] 48.24 2.18 (20) 1.19 (20) 4.8 (20) 1.11 [B] 1.7 (25)			, ,	, , ,		
Dibenzyl decanedioate 3.711 (25) 4.6 (25) 1.39 (21) [B] 38.2 (35) Dibenzyl ether o-Dibromobenzene m-Dibromobenzene p-Dibromobenzene p-Dibromobenzene 1,4-Dibromobutane 7.35 (20) 2.13 (20) [B] 3.80 (20) 1.5 (20) [B] 2.57 (95) 41.84 0.100 7 2.16 (20) [lq] 2.06 (20) [B] 2.20 (20) [B] 2	Dibenzylamine		3.6 (20)		43.27	0.108 6
decanedioate 3.711 (25) 1.39 (21) [B] 38.2 (35) o-Dibromobenzene 7.35 (20) 2.13 (20) [B] 38.2 (35) m-Dibromobenzene 3.80 (20) 1.5 (20) [B] 41.84 0.100 7 1,4-Dibromobutane 2.57 (95) 0 41.84 0.100 7 2,3-Dibromobutane 5.75 (25) 2.20 [g] 1.7 (25) [lq] 1,2-Dibromoethane 1.721 (20) 4.78 (25) 1.11 [g] 35.43 0.142 8 cis-1,2-Dibromoethylene 7.7 (0) 1.35 (B) 1.35 (B) 0 trans-1,2-Dibromoethylene 2.9 (0) 0 0	Dibenzyl		16(25)	1.02 (20) [B]		
Dibenzyl ether o-Dibromobenzene m-Dibromobenzene m-Dibromobenzene p-Dibromobenzene p-Dibromobenzene p-Dibromobutane 3.711 (25) 1.39 (21) [B] 2.13 (20) [B] 38.2 (35) 38.2 (35) p-Dibromobenzene p-Dibromobenzene p-Dibromobutane 1,4-Dibromobutane 2.57 (95) 0 41.84 0.100 7 2.16 (20) [Iq] 48.24 0.119 0 2,3-Dibromobutane 1,2-Dibromoethane moethylene trans-1,2-Dibromoethylene trans-1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1.721 (20) 4.78 (25) 1.11 [g] 1.35 (B) 7.70 (0) 2.88 (25) 35.43 0.142 8			4.0 (23)			
o-Dibromobenzene m-Dibromobenzene p-Dibromobenzene 1,4-Dibromobutane 7.35 (20) 3.80 (20) 2.57 (95) 2.13 (20) [B] 1.5 (20) [B] 41.84 41.84 0.100 7 0.119 0 2,3-Dibromobutane 1,2-Dibromoethane 1,2-Dibromoethylene trans-1,2-Dibromoethylene trans-1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1,2-Dibromoethylene 1.735 (20) 2.57 (95) 4.15 (20) [Iq] 1.77 (25) [Iq] 1.11 [g] 1.14 (20) [Iq] 7.77 (0) 1.35 (B) 0 35.43 0.142 8 1.35 (B) 0 0.142 8 0.142 8 0.142 8 1.35 (B) 0		3.711 (25)		1.39 (21) [B]	38.2.(35)	
m-Dibromobenzene p-Dibromobenzene 1,4-Dibromobutane 3.80 (20) 1.5 (20) [B] 41.84 0.100 7 1,4-Dibromobutane 1,4-Dibromobutane 2,3-Dibromobutane 5.75 (25) 2.20 [g] 48.24 0.119 0 2,3-Dibromobutane 2,3-Dibromoethane 2,3-Dibromoethane 2,3-Dibromoethylene 3,2-Dibromoethylene 4,2-Dibromoethylene 1,2-Dibromoethylene		(=0)	7.35 (20)		(00)	
1,4-Dibromobutane 2.16 (20) [lq] 2.06 (20) [B] 48.24 0.119 0 2,3-Dibromobutane 5.75 (25) 2.20 [g] 1.7 (25) [lq] 35.43 0.142 8 1,2-Dibromoethane actis-1,2-Dibromoethylene trans-1,2-Dibromoethylene 1,2-Dibromoethylene 1.286 (40) 4.09 (131) 1.14 (20) [lq] 1.35 (B) 1,2-Dibromoethylene 1,2-Dibromoethylene 2.88 (25) 0.142 8	m-Dibromobenzene			, , ,		
2,3-Dibromobutane 2,3-Dibromobutane 1.721 (20) 1.286 (40) 2.06 (20) [B] 2.20 [g] 1.7 (25) [Iq] 2.20 [g] 1.7 (25) [Iq] 35.43 0.142 8 1.286 (40) 4.09 (131) 1.14 (20) [Iq] 7.7 (0) 7.08 (25) 7.08 (25) 2.9 (0) 0 2.88 (25) 0 1.286 (25)	<i>p</i> -Dibromobenzene		2.57 (95)		41.84	0.1007
2,3-Dibromobutane 5.75 (25) 2.20 [g] 1,2-Dibromoethane 1.721 (20) 4.78 (25) 1.11 [g] 35.43 0.142 8 1.2-Dibromoethylene 7.7 (0) 1.35 (B) trans-1,2-Dibromoethylene 2.9 (0) 0 1,2-Dibromoethylene 2.88 (25)	1,4-Dibromobutane			2.16 (20) [lq]	48.24	0.1190
1.721 (20) 4.78 (25) 1.11 [g] 35.43 0.142 8 1.286 (40) 4.09 (131) 1.14 (20) [lq] 1.35 (B) 7.08 (25) 2.9 (0) 2.88 (25) 1.2-Dibro-moethylene 1,2-Dibro-moethylene 1,2-Dibro-moethy						
1,2-Dibromoethane 1.721 (20) 4.78 (25) 1.11 [g] 35.43 0.142 8 cis-1,2-Dibromoethylene 7.7 (0) 1.35 (B) trans-1,2-Dibromoethylene 2.9 (0) 0 1,2-Dibromoethylene 2.88 (25)	2,3-Dibromobutane		5.75 (25)			
cis-1,2-Dibromoethylene 1.286 (40) 4.09 (131) 1.14 (20) [lq] 7.7 (0) 1.35 (B) 7.08 (25) 2.9 (0) 0 2.88 (25) 0						
cis-1,2-Dibromoethylene 7.7 (0) 1.35 (B) trans-1,2-Dibromoethylene 7.08 (25) moethylene 2.9 (0) 0 1,2-Dibromoethylene 2.88 (25)	1,2-Dibromoethane				35.43	0.1428
moethylene 7.08 (25) trans-1,2-Dibro- moethylene 1,2-Dibro- 1,2-Dibro- 7.08 (25) 2.9 (0) 0 2.88 (25)	.:. 1 2 Dib	1.286 (40)				
trans-1,2-Dibromoethylene 2.9 (0) 0 1,2-Dibromoethylene 2.88 (25)				1.33 (B)		
moethylene 2.88 (25) 1,2-Dibro-	•			0		
, , , , , , , , , , , , , , , , , , , ,				J		
moheptane 3.8 (25) 1.78 (25) [D]	,					
	moheptane		3.8 (25)	1.78 (25) [D]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
2,3-Dibro-		5.1 (25)	2.15 (25) [B]		
moheptane 3,4-Dibro-		4.7 (25)	2.15 (25) [B]		
moheptane		4.7 (23)	2.13 (23) [B]		
Dibromomethane		7.77 (10)	1.43 [g]	42.77	0.148 8
Dioromomethane		6.7 (40)	1.45 (20) [lq]	72.77	0.1400
1,2-Dibromo-	1.5 (25)	4.3 (20)	1.43 (25) [B]	36.81	0.115 5
propane Dibromotetra-	0.72 (25)	2.34 (25)		18.9 (20)	18.1 (25)
fluoroethane	, ,			\	. ,
Dibutylamine	0.95 (20)	2.978 (20)	1.06 (20) [lq]	26.50	0.095 2
			1.05 (20) [B]		
Dibutyl	9.03 (25)	4.54 (30)	2.64 (25) [B]		
decanedioate					
Dibutyl ether	0.602 (30)	3.06 (25)	1.18 [g]	24.78	0.093 4
			1.19 (20) [lq]		
Dibutyl maleate	5.62 (20)		2.70 (25) [B]	32.46	0.086 5
0 (D') (1) 1	4.76 (25)		1 (0 (20) FD1		
2,6-Di- <i>tert</i> -butyl-	3.47 (80)		1.68 (20) [B]		
4-methylphenol Dibutyl	19.91 (20)	6.436 (30)	2.07.(20) [[-1	22.40.(20)	
<i>o</i> -phthalate	7.85 (45)	5.99 (45)	2.97 (20) [lq] 2.85 (30) [B]	33.40 (20)	
Dichloroacetic	3.23(50)	8.2 (22)	2.83 (30) [B]	37.8	0.0927
acid	1.92 (75)	7.8 (61)		37.6	0.072 7
o-Dichlorobenzene	1.324 (25)	9.93 (25)	2.51 [g]	26.84 (20)	35.55 (30)
o Bremorocement	1.02 (20)	7.10 (90)	2.26 (24) [B]	2010 1 (20)	20.00 (00)
m-Dichlorobenzene	1.045 (23)	5.04 (25)	1.68 [g]	38.30	0.1147
	0.955 (33)	4.22 (90)	1.38 (24) [B]		
<i>p</i> -Dichlorobenzene	0.839 (55)	2.41 (50)	0	34.66	0.0879
	0.668 (79)				
1,4-Dichlorobutane		8.9 (25)	2.22 [g]	37.79	0.1174
			2.13 (25) [lq]		
Dichlorodifluoro-	0.26 (25)	2.13 (29)	0.51 [g]	9 (25)	
methane	0.013 (25) [g]				
1,1-Dichloroethane	` '	10.1 (18)	2.06 [g]	27.03	0.1186
100'11 4	0.430 (30)	10.86 (16)	2.00 (25) [B]	25.42	0.142.0
1,2-Dichloroethane	0.887 (15)	12.7 (-10)	1.48 [g]	35.43	0.1428
1,1-Dichloroe-	0.730 (30)	10.65 (20)	1.7 (20) [B]		
thylene	0.442 (0) 0.358 (20)	4.67 (16)	1.30 (25) [B]		
cis-1,2-Dichlo-	0.338 (20)	9.20 (25)	2.95 [g]	28 (20)	
roethylene	0.444 (25)	7.20 (23)	1.90 (25) [B]	20 (20)	
trans-1,2-Dichlo-	0.423 (15)	2.14 (25)	0.70 (25) [B]	25 (20)	
roethylene	0.404 (20)	(25)	5 0 (2 5) [D]	25 (20)	
	- (/				

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
2,2'-Dichloro- ethyl ether	2.41 (20) 2.065 (25)	21.2 (20)	2.61 (20) [B]	40.57	0.1306
Dichlorofluoro- methane	0.34 (25) 0.011 (25) [g]	5.34 (28)	1.3 [g]	18 (25)	
Dichloromethane	0.449 (15) 0.393 (30)	9.14 (20) 1.006 5 (100)	1.60 [g] 1.90 (20) [B]	30.41	0.1284
2,4-Dichloro- phenol	0.373 (30)	[g]	1.60 (25) [B]	46.59	0.1221
1,2-Dichloro- propane	0.865 (20) 0.700 (25)	8.925 (26) 7.90 (35)	1.87 (25) [B]	31.42	0.1240
1,3-Dichloro- propane	0.700 (23)	7.50 (55)	2.08 [g] 2.2 (25) [B]	36.40	0.123 3
2,2-Dicloro- propane 1,1-Dichloro-2-	0.769 (15) 0.619 (30)	11.37 (20) 14 (20)	2.62 [g] 2.20 (25) [B]	23.60 (20)	22.53 (30)
propanone 1,2-Dichlorotetra- fluoroethane	0.38 (25)	2.26 (25)	0.53 [g]	12 (25)	
α, α -Dichloro-	0.011 (25) [g]	6.9 (20)	2.07 (20) [B] 2.05 (25) [B]	41.26	0.103 5
Diethanolamine	368 (30) 196 (40)	2.81 (25)	2.84 (25) [B]		
1,1-Diethoxyethane 1,2-Diethoxyethane		3.80 (25)	1.08 [g] 1.99 (20) [B] 1.65 (25) [B]	23.46	0.103 0
Diethoxymethane			(.)[]	23.87	0.129 1
Diethylamine	0.388 (10) 0.273 (38)	3.6 (22)	0.92 [g] 1.11 (25) [lq]	22.71	0.1143
N, N-Diethy- laniline	1.15 (30) 0.750 (75)	5.5 (19)	1.40 (20) [lq] 1.80 (20) [B]	36.59	0.1040
Diethyl carbonate	0.868 (15) 0.748 (25)	2.82 (20)	1.07 [g] 0.91 (25) [B]	28.62	0.1100
Diethyl decanedioate		5.0 (30)	2.38 (20) [lq] 2.52 (20) [B]	34.68	0.0959
Diethyl ether	0.247 (15) 0.245 (20)	4.335 (20) 3.97 (40)	1.15 [g] 1.22 (16) [lq]	18.92	0.0908
Diethyl ethyl phosphonate Diethyl fumarate	1.627 (15) 0.969 (45)	11.00 (15) 9.86 (45) 6.5 (23)	2.95 (32) [lq] 2.91 (20) [C] 2.40 (20) [B]	30.63	0.097 5
Diethyl glutarate Di(2-ethylhexyl)-	6.00 (45)	6.7 (30) 4.09 (45)	2.46 (30) [lq]	34.34	0.101 0
2-ethylhexyl- phosphonate	3.61 (65)	3.94 (65)			
Di(2-ethylhexyl) o-phthalate	33.67 (35) 21.40 (45)	4.91 (35) 4.77 (45)			

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface t	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Diethyl maleate	3.57 (20) 3.14 (25)	8.58 (23)	2.56 (25) [B]	34.67	0.103 9
Diethyl malonate	2.15 (20) 1.94 (25)	8.03 (25)	2.49 (20) [lq] 2.54 (25) [B]	33.91	0.104 2
Diethyl		5.13 (30)			
nonanedioate Diethyl oxalate	2.311 (15) 1.618 (30)	8.1 (21)	2.49 (20) [D]	34.32	0.1119
Diethyl o-phthalate	9.18 (35) 6.41 (45)	7.34 (35) 7.13 (45)	2.8 (25) [B]	38.47	0.0963
Diethyl succinate		6.64 (30)	2.3 [g] 2.37 (30) [lq]	33.97	0.104 1
Diethyl sulfate		29 (20)	4.46 (25) [D]	35.47	0.0976
Diethyl sulfide Diethyl sulfite	0.446 (20) 0.422 (25)	5.72 (25) 5.24 (50) 16 (20)	1.52 [g] 1.58 (20) [B]	27.33	0.1106
Diethylzinc		14 (50) 2.5 (20)	0.62 (25) [B]		
1,1-Difluoroethane 1,2-Dihydroxy- benzene	0.243 (21)	2.30 [g] 2.6 (-89)	2.60 (25) [B]	47.6	0.084 9
1,3-Dihydroxy- benzene		3.2 (18)	2.09 (44) [B]	54.8	0.071 7
1,4-Dihydroxy- benzene			1.4 (44) [B]		
1,2-Diiodobenzene		5.7 (20)	1.70 (20) [B]		
1,3-Diiodobenzene		4.3 (25)	1.22 (20) [B]		
1,4-Diiodobenzene		2.9 (120)	0.19 (20) [B]		
cis-1,2-Diiodo- ethylene		4.46 (83)	0.71 [B]		
trans-1,2-Diiodo- ethylene		2.19 (83)	0		
Diiodomethane	3.043 (15) 2.392 (30)	5.316 (25)	1.08 (25) [B]	70.21	0.161 3
Diisobutylamine Diisobutyl <i>o</i> -phthalate	30 (20)	2.7 (22)	1.10 (25) [B]	24.00	0.091 2
Diisopentylamine		2.5 (18)	1.48 (30) [B]	26.04	0.085 8
Diisopentyl ether	1.40 (11) 1.012 (20)	2.82 (20)	0.98 (20) [lq] 1.23 (25) [B]	24.76	0.087 1
Diisopropylamine	0.40 (25)		1.26 (25) [B]	21.83	0.107 7
Diisopropyl ether	0.379 (25)	3.88 (25)	1.13 [g] 1.26 (25) [B]	19.89	0.104 8
1,2-Dimethoxy- benzene	3.281 (25) 2.184 (40)	4.09 (25)	1.32 (25) [B]	34.4	0.064 2

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

		5.1	5	Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
1,1-Dimetho- xyethane				23.90	0.1159
1,2-Dimetho- xyethane	0.530 (10) 0.455 (25)	7.60 (10) 7.20 (25)	1.71 (25) [B]	48.0 (25)	
Dimethoxy- methane	0.340 (15) 0.325 (20)	2.65 (20)	0.74 [g]	23.59	0.1199
N,N-Dimethy lacetamide	2.141 (20) 0.838 (30)	37.78 (25)	3.80 [g] 4.60 (20) [lq]	32.43 (30)	29.50 (50)
Dimethylamine	0.207 (15) 0.186 (25)	6.32 (0) 5.26 (25)	1.03 [g] 1.14 (25) [lq]	29.50	0.126 5
N,N-Dimethy-laniline	1.285 (25) 0.91 (50)	4.9 (20) 4.4 (70)	1.61 [g] 1.55 (25) [B]	38.14	0.1049
2,4-Dimethy- laniline			1.40 (25) [B]	39.34	0.0996
2,2-Dimethyl- butane	0.351 (25) 0.330 (30)	1.873 (25)	0	18.29	0.0990
2,3-Dimethyl- butane	0.361 (25) 0.342 (30)	1.890 (25)	0	19.38	0.1000
2,3-Dimethyl-1- butanol				26.22	0.099 2
N,N-Dimethyl- butyramide	1.271	2.00			
Dimethyl carbonate			0.90 [g] 0.96 (25) [B]	31.94	0.1343
1,1-Dimethyl- cyclopentane 2,2-Dimethyl-1,			0	23.78	0.101 6
3-dioxolane- 4-methanol	11 (20)				
Dimethyl ether	0.0104 (60)	5.02 (25) 2.97 (110)	1.30 [g] 1.25 (25) [B]	14.97	0.147 8
<i>N,N</i> -Dimethyl-formamide	0.845 (20) 0.598 (50)	38.3 (20) 36.71 (25)	3.86 (25) [B]	36.76 (20)	34.40 (40)
2,4-Dimethyl- heptane	0.370 (30)	1.9 (20)	0	23.21	0.0929
2,5-Dimethyl- heptane		1.9 (20)	0	23.21	0.0929
2,6-Dimethyl- heptane		2 (20)	0	22.77	0.0887
2,6-Dimethyl-4- heptanone	1.03 (20)		2.66 (25) [C]		
Dimethyl hexanedioate	14 (20)		2.28 (20) [B]	38.26	0.1138
Dimethyl hydrogen	1.08 (25)				
phosphonate					

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Dimethyl maleate	3.54 (20) 3.21 (25)		2.48 (25) [C]	40.73	0.122 0
Dimethyl					
malonate		10 (20)	2.41 (20) [B]	39.72	0.1208
2,2-Dimethyl-		1.91 (20)	0	19.94	0.095 7
pentane					
2,3-Dimethyl-	0.406 (20)	1.939 (20)	0	21.96	0.099 5
pentane	0.261 (20)	1.014 (20)		20.00	0.007.2
2,4-Dimethyl- pentane	0.361 (20)	1.914 (20)	0	20.09	0.097 2
3,3-Dimethyl-		1.94 (20)	0	21.59	0.0996
pentane		1.94 (20)	U	21.39	0.0990
2,4-Dimethyl-			1.48 (20) [B]	34.57	0.0869
phenol			1.98 (60) [B]		
2,5-Dimethyl-	1.55 (80)		1.43 (20) [B]	36.72	0.0850
phenol	, ,		1.52 (60) [B]		
3,4-Dimethyl-	3.00 (80)	4.8 (17)	1.77 (20) [B]	35.75	0.0910
phenol					
3,5-Dimethyl-	2.42 (80)		1.76 (20) [B]	34.09	0.0807
phenol	15.0 (05)	0.05 (0.5)	20(25) 573		
Dimethyl	17.2 (25)	8.25 (25)	2.8 (25) [B]		
o-phthalate	6.41 (45)	8.11 (45)	0	12.05 (20)	10.09 (20)
2,2-Dimethyl- propane	0.328 (0) 0.303 (5)	1.80 (20) 1.678 (98)	U	12.03 (20)	10.98 (30)
N,N-Dimethyl-	0.935	33.1			
propionamide	0.755	33.1			
2,5-Dimethyl-		2.43 (20)	0		
pyrazine					
2,3-Dimethyl-		2.3 (25)	0		
quinoxaline					
Dimethyl		5.1 (20)	2.09 (20) [B]	39.00	0.1191
succinate					
Dimethyl sulfate		48.3 (20)	4.31 (25) [D]	41.26	0.1163
D: 1 1 101	0.200 (20)	46.4 (20)	1 45 (05) FD1	26.07	0.000.5
Dimethyl sulfide	0.289 (20)	6.2 (20)	1.45 (25) [B]	26.07	0.080 5
Dimathyl sulfita	0.265 (36)	22.5 (23)	2.02.(20) [B]	36.48	0.125 3
Dimethyl sulfite	0.715 (30) 0.436 (80)	22.3 (23)	2.93 (20) [B]	30.46	0.123 3
Dimethyl	2.47 (20)	48.9 (20)	3.9 (25) [B]	43.54 (20)	42.41 (30)
sulfoxide	1.192 (55)	41.9 (55)	3.5 (23) [B]	43.54 (20)	42.41 (30)
2,4-Dimethyl-	1 ()	(==,			
tetrahydrothi-					
ophene-1, 1-					
dioxide	9.04	29.5			

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface tension, dyn·cm ⁻¹	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
N,N-Dimethyl- o-toluidine		3.4 (20)	0.88 (25) [B]		
N,N-Dimethyl- p-toluidine		3.9 (20)	1.29 (25) [B]		
Dinonyl hexanedioate	37 (20)		2.53 (25) [B]		
Dinonyl o-phthalate		4.65 (35) 4.52 (45)			
Dioctyl decanedioate		4.0 (27)			
Dioctyl o-phthalate		5.1 (25)	3.06 (25) [C]		
1,4-Dioxane	1.439 (15) 1.087 (30)	2.24 (20) 2.21 (25)	0	36.23	0.139 1
Dipentyl ether	1.188 (15) 0.922 (30)	2.77 (25)	0.98 (20) [lq] 1.24 (25) [B]	26.66	0.092 5
Dipentyl o-phthalate	17.03 (35) 11.51 (45)	5.79 (35) 5.62 (45)	2.71 (20) [lq]	32.56	0.073 9
Dipentyl sulfide Diphenylamine	4.66 (55) 1.04 (130)	3.83 (25) 3.3 (52)	1.59 (25) [B] 1.31 (20) [C] 1.01 (25) [B]	29.55 45.36	0.087 6 0.101 7
1,2-Dipheny- lethane		2.4 (110)	0 (110) [lq] 0.45 (25) [B]		
Diphenyl ether	2.61 (40) 2.09 (50)	3.65 (30)	1.16	28.70	0.078 0
Diphenylmethane		2.7 (18) 2.57 (26)	0.26 (30) [lq] 0.3 (25) [B]		
1,1-Dipropo- xyethane				25.03	0.097 2
Dipropo- xymethane				25.17	0.095 3
Dipropylamine	0.534 (20) 0.427 (37)	3.07 (20)	1.01 (20) [lq] 1.03 (20) [B]	24.86	0.102 2
Dipropyl carbonate				28.94	0.101 5
Dipropylene glycol butyl ether	4.23 (25)			28.2 (25)	
Dipropylene glycol ethyl	3.11 (25)			27.7 (25)	
ether Dipropylene glycol isopropyl ether	386 (25)			25.9 (25)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to dyn·ci	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Dipropylene glycol methyl ether	3.1 (25)			28.8 (25)	
Dipropyl ether Divinyl ether	0.448 (15) 0.376 (30)	3.39 (26) 3.9 (20)	1.21 [g] 1.17 (30) [H] 1.07 (20) [lq]	22.60	0.1047
Dodecamethyl- cyclohexasil- oxane		2.6 (20)	1.07 (20) [iq]		
Dodecamethyl- pentasiloxane		2.5 (20)		17.08 (25)	
Dodecane	1.508 (20) 1.378 (25)	2.05 (-10) 2.01 (20)	0	27.12	0.0884
1-Dodecanol		5.15 (20) 6.5 (25)	1.52 (20) [B]	31.25	0.0748
6-Dodecyne		2.17 (25)			
1,2-Epoxybutane	0.41 (20) 0.40 (25)		2.01 (20) [B]	23.9 (20)	
Erythritol		28 (128)			
Ethane [g]	0.009 0 (20) 0.011 4 (100)	1.001 5 (0)	0	1.24	0.166 0 [lq]
1,2-Ethanedia- mine	1.54 (20) 1.226 (30)	16.8 (18) 14.2 (20)	1.96 [g] 1.92 (25) [B]	44.77	0.1398
1,2-Ethanediol	26.09 (15) 13.55 (30)	38.66 (20) 37.7 (25)	2.28 [g] 2.3 (25) [D]	50.21	0.0890
1,2-Ethanediol diacetate	3.13 (20)	13 (30)	2.34 (30) [B]		
Ethanesulfonic acid				45.74	0.0824
Ethanesulfonyl chloride			3.89 (25) [B]	43.43	0.1177
Ethanethiol	0.003 16 [g]	6.9 (15)	1.57 [g] 1.40 (20) [B]	25.06	0.079 3
Ethanol	1.209 (19) 0.991 (30)	25.00 (20) 20.21 (55)	1.69 [g] 1.71 (25) [B]	24.05	0.083 2
Ethoxybenzene	1.364 (15) 1.040 (30)	4.22 (20)	1.41 [g] 1.36 (25) [CS ₂]	35.17	0.1104
2-Ethoxyethanol	2.04 (20) 1.85 (25)	29.6 (24)	2.24 (30) [B]	30.59	0.0897
2-(2-Ethoxyeth- oxy)ethanol	3.71 (25)			31.8 (25)	27.2 (75)
2-Ethoxyethyl acetate	1.025 (25)	7.567 (30)	2.25 (30) [B]	31.8 (25)	

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	,
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
1-Ethoxy-2- methylbutane		3.96 (20)			
1-Ethoxynaph- thalene		3.3 (19)			
1-Ethoxypentane		3.6 (23)			
1-Ethoxy-2- propanol	1.68 (25)			25.9 (25)	
α -Ethoxytoluene		3.9 (20)			
Ethyl acetate	0.473 (15)	6.11 (20)	1.78 [g]	26.29	0.116 1
Ethyl	0.426 (25) 1.419 (20)	5.30 (77) 15.7 (22)	1.84 (25) [lq] 3.22 (18)	34.42	0.1015
acetoacetate	1.508 (25)	13.7 (22)	[B keto form] 2.04 (-80) [CS ₂ , enol form]	37.72	0.1013
Ethylamine		6.94 (10)	1.40 (25) [B]	22.63	0.137 2
2-(Ethylamino) ethanol	12.40 (25)	0.5 1 (10)	11.10 (20) [2]	22.00	0.157.2
N-Ethylaniline	2.04 (25) 1.08 (55)	5.76 (20)		39.00	0.1070
Ethylbenzene	0.669 (20) 0.531 (40)	2.41 (20)	0.37 (25) [lq]	31.48	0.1094
Ethyl benzoate	2.407 (15) 1.751 (30)	6.02 (20)	1.95 [g] 1.93 (25) [B]	37.16	0.1059
Ethyl α - bromobutyrate		8 (20)	2.40 (25) [B]		
2-Ethyl-1-butanol	8.021 (15) 5.892 (25)	6.19 (90)		25.06 (15)	24.32 (25)
Ethyl butyrate	0.771 (15) 0.613 (25)	5.10 (18)	1.74 (22) [B]	26.55	0.1045
2-Ethylbutyric acid	3.3 (20)			26.3 (20)	
Ethyl carbamate	0.916 (105) 0.715 (120)	14.2 (50)	2.59 (30) [D]		
Ethyl chloroacetate		11.4 (21)	2.65 (25) [B]	34.18	0.1177
Ethyl chloroformate		11 (20)	2.56 (35) [B]	28.90	0.108 4
Ethyl cinnamate	8.7 (20)	6.1 (18)	1.86 (20) [B]	39.99	0.104 5
Ethyl crotonate	2.056 (15)	5.4 (20)	1.95 (24) [B]	29.31	0.1066
Ethyl	3.256 (15)	26.9 (20)	4.04 (30) [B]	38.80	0.109 2
cyanoacetate Ethylcyclohexane	2.148 (30) 0.843 (20) 0.787 (25)	2.054 (20)	0 [g]	27.78	0.105 4
Ethyl dichloroacetate	(-2)	12 (2) 10 (22)	2.63 (25) [B]	34.89	0.115 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
N-Ethyldie- thanolamine	53 (25)				
Ethyl dodecanoate		3.4 (20) 2.7 (143)	1.3 (20) [lq]	30.05	0.0863
Ethylene Ethylene carbonate	1.85 (40)	1.001 44 (0) 89.6 (40) 69.4 (91)	0 [g] 4.87 (25) [B]	-2.7	0.185 4
Ethylenediamine	1.540 (18)	16.0 (18) 14.2 (20)	1.98 [g] 1.92 (25) [B]	44.77	0.1398
Ethylene dinitrate 2,2'-(Ethylenedioxy)diethanol	38 (20)	28.3 (20) 23.69 (20)	3.58 (25) [B] 5.58 [lq]	49.1 (0) 47.33	46.7 (45) 0.088 0
Ethylene glycol	26.09 (15) 13.35 (30)	41.2 (20) 37.7 (25)	2.27 [g] 2.20 (15) [lq]	50.21	0.089 0
Ethylene oxide	0.3 (0)	14 (-1)	1.88 [g] 1.92 (20) [lq]	27.66	0.1664
Ethyleneimine	0.418 (25)	18.3 (25)	1.89 [g] 1.77 (25) [B]	7.9 (20)	0.424.7
Ethyl formate	0.419 (15) 0.358 (30)	7.16 (25)	1.94 [g] 1.96 (25) [lq]	26.47	0.131 5
Ethyl fumarate Ethyl hexadecanoate 2-Ethyl-1, 3-	323 (20)	6.5 (23) 3.2 (20) 2.71 (104)	1.2 [lq]	33.90 32.86	0.105 6 0.085 9
hexanediol Ethyl hexanoate 2-Ethylhexanoic	7.7 (20)		1.80 (20) [B]	27.73	0.0960
acid 2-Ethyl-1-hexanol 2-Ethylhexyl	9.8 (20) 1.5 (20)	4.41 (90)	1.74 (25) [B]	30.0 (22)	
acetate Ethyl isobutyrate Ethyl isopentyl ether		3.96 (20)		25.33	0.104 6
Ethyl isothio- cyanate		19.5 (21)	3.67 (20) [B]	38.69	0.1326
Ethyl lactate Ethyl maleate	2.44 (25)	13.1 (25) 8.6 (23)	2.4 (20) [B]	30.72	0.0983
Ethyl 3- methylbutyrate		4.71 (18)		25.79	0.1006
Ethyl methyl ether			1.22 [g]	18.56	0.1317
Ethyl methyl sulfide	0.373 (20) 0.354 (25)			27.63	0.128 6
Ethyl nitrate		19.4 (20)	2.93 (20) [B]	30.81	0.134 5

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Ethyl 9-		3.2 (25)	1.83 (20) [lq]		
octadecenoate		10 (01)			
Ethyl 4-		12 (21)			
oxopentanoate		1.04 (20)		22.52	0.102.2
3-Ethylpentane	0.947 (20)	1.94 (20)	0 1.76 (28) [D]	22.52 27.15	0.103 2 0.099 9
Ethyl pentanoate Ethyl pentyl ether	0.847 (20)	4.7 (18)	1.76 (28) [B]	24.19	0.099 9
Ethyl phenylacetate	5.3 (21)	3.6 (23) 1.82 (30)	1.2 (20) [B]	24.19	0.099 2
Ethyl phenyl	3.3 (21)	1.62 (30)	4.08 (25) [B]	39.30	0.113 1
sulfide			4.08 (23) [D]	39.30	0.113 1
Ethyl propionate	0.564 (15)	5.65 (19)	1.75 (22) [B]	26.72	0.1168
Linyi propionate	0.473 (30)	3.03 (17)	1.73 (22) [B]	20.72	0.1100
Ethyl propyl ether	0.323 (20)		1.16 (25) [B]	21.92	0.1054
Euryr propyr curer	0.225 (60)		1.10 (23) [B]	21.72	0.105 4
Ethyl salicylate	1.772 (45)	7.99 (30)	2.85 (25) [B]	31.00	0.109 1
Ethyl stearate	11,72(10)	2.98 (40)	1.65 (40) [lq]	21.00	0.1071
		2.69 (100)	(10)[14]		
Ethyl thiocyanate		29.3 (21)	3.33 (20) [B]	37.28	0.1226
o-Ethyltoluene			(1/1]	32.33	0.1060
<i>p</i> -Ethyltoluene		2.24 (25)	0	30.98	0.107 5
Ethyl		7.8 (20)	2.56 (25) [B]	32.97	0.1073
trichloroacetate					
Ethyl vinyl ether	0.2		1.26 (20) [B]	19.00 (20)	
Ethynyl acetate				32.81 (20)	30.20 (40)
Fluorobenzene	0.620(15)	5.42 (25)	1.61 [g]	29.67	0.1204
	0517 (30)	4.7 (60)	101 [8]	-,,,,	
1-Fluorohexane				23.41	0.100 1
2-Fluoro-2-		5.89 (20)	1.92 (25) [B]		
methylbutane					
1-Fluoropentane		4.24(20)	1.85 (25) [B]	22.81	0.1315
o-Fluorotoluene	0.680(20)	4.22 (30)	1.35 [g]		
	0.601 (30)	3.9 (60)	1.26 (30) [lq]		
m-Fluorotoluene	0.608 (20)	5.42 (30)	1.86 [g]	32.31	0.1257
	0.534 (30)	4.9 (60)	1.66 (30) [lq]		
<i>p</i> -Fluorotoluene	0.622 (20)	5.86 (30)	2.00 [g]	30.44	0.1109
	0.522 (30)	5.3 (60)	1.76 (30) [lq]		
Formamide	4.320 (15)	111.0 (20)	3.73 [g]	59.13	0.084 2
	2.296 (30)	103.5 (40)			
Formanilide	1.65 (120)		3.37 (25) [C]	44.30	0.087 5
Formic acid	1.966 (15)	58.5 (15)	1.35 [g]	39.87	0.1098
A.D. 1111	1.219 (40)	57.0 (21)	1.20 (25) [B]		0.425 =
2-Furaldehyde	2.475 (0)	41.9 (20)	2.13 (25) [lq]	46.41	0.1327
P.	1.494 (25)	34.9 (50)	3.63 (25) [B]	24.10.(20)	22 20 (25)
Furan	0.380 (20)	2.95 (25)	0.66 [g]	24.10 (20)	23.38 (25)
	0.361 (25)		0.67 (20) [B]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Furfuryl alcohol	4.62 (25)		1.92 (25) [lq]	ca 38 (20)	
Glycerol	945 (25) 134 (50)	42.5 (25)	2.68 (25) [D]	63.14 (17)	62.5 (25)
Glycerol triacetate		7.2 (20)	2.73 (25) [B]	37.88	0.081
Glycerol trinitrate	36.0 (20) 13.6 (40)	19 (20)	3.38 (25) [B]	55.74	0.2504
Glycerol trioleate		3.2 (26)	3.11 (23) [B]	36.03	0.0699
Glycerol tripalmitate		2.9 (65)	2.80 (23) [B]	32.26	0.067 2
Glycerol tristearate		2.8 (70)	2.86 (23) [B]	32.73	0.068 5
Heptanaldehyde	0.977 (15)	9.1 (20)	2.26 (40) [lq] 2.58 (22) [B]	28.64	0.0920
Heptane	0.416 (20) 0.341 (40)	1.924 (20) 1.85 (70)	0	22.10	0.0980
Heptanoic acid	3.40 (30)	2.6 (71)		29.88	0.0848
1-Heptanol	7.014 (20) 8.53 (15)	12.1 (22)	1.73 (20) [B]		
DL-2-Heptanol	5.06 (25)	9.21 (22)	1.73 (20) [B]		
DL-3-Heptanol		6.9 (22)	1.73 (20) [B]		
4-Heptanol		6.2 (22)	1.72 (20) [B]		
2-Heptanone	0.854 (15)	11.95 (20)	2.61 (22) [B]	28.76	0.105 6
3-Heptanone	0.686 (30)	8.27 (100) 12.9 (22)	2.81 (22) [B]	28.24	0.1015
4-Heptanone	0.736 (20)	12.60 (20)	2.74 (20) [B]	28.11	0.1013
·		9.46 (80)	() []		
1-Heptene	0.35 (20) 0.34 (25)	2.07 (20)	0.34 (20) [lq]	22.28	0.099 1
Hexadeca- methylcyclo- octasiloxane		2.7 (20)			
Hexadecane	3.591 (22)		0	29.18	0.085 4
1-Hexadecanol		3.8 (50)	1.67 (25) [B]		
1,5-Hexadiene	0.275 (20) 0.244 (36)				
2,4-Hexadiene Hexafluoro- benzene		2.2 (25)	0.31 (25) [B] 0	22.6 (20)	
Hexamethyl- disiloxane		2.2 (20)	0.37 (25) [lq]	17.01	0.0763
Hexamethyl- phosphoramide	3.47 (20)	30 (20)	4.31 (25) [lq]	33.8 (20)	
Hexane	0.313 (20) 0.271 (40)	1.904 (15) 1.890 (20)	0	20.44	0.102 2
Hexanedinitrile	5.99	32.45	3.8 (25) [B]	47.88	0.0973

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

ace tension, yn·cm ⁻¹					
b	а	Dipole moment, D	Dielectric constant, ε	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Substance
0.100 2	32.22				2,4-Hexanedione
	29.64		17.26 (25)	1.041 (15)	Hexanenitrile
			, ,	0.830 (30)	
(20) 27.55 (25)	28.05 (20)	1.13 (25) [lq]	2.63 (71)	3.525 (15)	Hexanoic acid
	`			2.511 (3)	
0.080 1	27.81	1.55 (20) [B]	13.3 (25)	6.203 (15)	1-Hexanol
			8.5 (75)	3.872 (30)	
0.109 2	28.18	2.68 (22) [B]	14.6 (15)	0.584 (25)	2-Hexanone
0.102 7	20.47	0.34 (20) [lq]	2.051 (20)	0.26 (20)	1-Hexene
				0.25 (25)	
0.097 0	28.44				Hexyl acetate
20)	31.0 (20)	3.24 (20) [B]	18.2 (25)	2.9 (25)	4-Hydroxy-4-
					methyl-2-
					pentanone
0.1123	41.52	1.71 [g]	4.62 (20)	1.774 (17)	Iodobenzene
		1.3 (20) [B]		0.488 (149)	
0.013 1	30.82	2.10 [g]	6.22 (20)		1-Iodobutane
		1.90 (20) [B]	4.52 (130)		
0.105 6	30.32	2.06 (20) [B]			2-Iodobutane
		1.87 (20) [C]	3.9 (20)		1-Iodododecane
0.128 6	31.67	1.91 [g]	10.2(-50)	0.617 (15)	Iodoethane
		1.69 (20) [lq]	7.82 (20)	0.540 (30)	
0.088 7	32.18	1.86 (22) [B]	4.9 (22)		1-Iodoheptane
		1.95 (22) [B]	6.4 (22)		3-Iodoheptane
	34.49		3.5 (20)		1-Iodohexadecane
	31.63	1.94 (20) [C]	5.37 (20)		1-Iodohexane
0.123 4	33.42	1.64 [g]	7.00 (20)	0.500 (20)	Iodomethane
0.001.5	20.27	1.42 (20) [B]	5.6.(10)	0.424 (40)	1 7 1 2
0.091 5	30.37	1.85 (20) [B]	5.6 (19)		1-Iodo-3-
		2 20 (20) FD1	0.10 (20)		methylbutane
		2.20 (20) [B]	8.19 (20)		2-Iodo-2- methylbutane
0.017 2	20.26	1.90 (20) [D]	6.5 (20)	0.975 (20)	•
0.0172	30.20	1.89 (20) [D]	0.3 (20)	` '	
0.091 5	32.51	1 80 (25) [[a]	16 (25)	0.097 (40)	
0.0713	32.31	. , . 13	4.0 (23)		1-10dooctane
			5.8 (20)		2-Indooctane
0.1014	31 41	. ,	` /		
0.113 6	1			0.837 (15)	
0.115 0	21.01	103	, (20)	\ /	. 10dopropune
0.1107	29.35	. ,	7.87 (20)	` '	2-Iodopropane
	100	(==, [=]		` '	rr
0.096 5	39.23	1.72 (22) [B]	4.4 (35)		<i>p</i> -Iodotoluene
	34.10		11 (18)		α -Ionone
0.095 0	35.36		12 (20)		β -Ionone
	39.23 34.10	1.89 (20) [B] 1.80 (25) [Iq] 1.90 (20) [C] 2.07 (20) [C] 1.90 (20) [B] 2.03 [g] 1.86 (20) [B] 2.01 (20) [B] 1.72 (22) [B]	11 (18)	0.875 (20) 0.697 (40) 0.837 (15) 0.670 (30) 0.732 (15) 0.620 (30)	α -Ionone

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	,
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Iron pentacarbonyl		2.6 (20)			
Isobutyl acetate		5.29 (20)	1.87 (22) [B]	25.59	0.101 3
Isobutylamine	0.553 (25)	4.43 (21)	1.27 (25) [B]	24.48	0.109 2
Isobutylbenzene		2.319 (20)	0.31 (20) [lq]	29.39	0.096 1
T 1 1 1		2.298 (30)		24.47	0.004.2
Isobutyl formata	0.680 (20)	4.1 (20)	1.90 (20) FB1	24.47	0.084 3 0.112 2
Isobutyl formate Isobutyl	0.680 (20)	6.41 (19)	1.89 (20) [B]	26.14 30.92	0.112 2 0.127 0
isobutyrate		2.7 (20)			
Isobutyl nitrate		2.7 (20)			
Isobutyl pentanoate Isobutyl		3.8 (19)		28.97	0.1166
propionate				20.97	0.1100
Isobutyric acid	1.44 (15)	2.7 (20)	1.09 (25) [lq]	26.88	0.0920
Isobutyric anhydride	14 (20)	2.7 (20)	1.05 (23) [14]	20.00	0.072 0
Isobutyronitrile	0.551 (15) 0.456 (30)	20.4 (24)	3.61 (25) [B]	24.93 (20)	23.84 (30)
Isopentyl acetate	0.872 (20)	4.81 (20)	1.84 (22) [B]	26.75	0.0989
	0.790 (25)	4.63 (30)	1.76 (30) [lq]		
Isopentyl butyrate	, ,	4.0 (20)	. , , , ,	27.32	0.0918
Isopentyl		3.6 (19)	1.8 (28) [B]		
pentanoate					
Isopentyl	4.2 (20)				
propionate					
Isopropyl acetate	0.559 (20)		1.86 (22) [B]	24.44	0.107 2
Isopropylamine	0.36 (25)	5.45 (20)	1.45 (25) [B]	19.91	0.097 2
Isopropylbenzene	0.791 (20)	2.39 (20)	0.65 [g]	30.32	0.105 4
T1 f	0.739 (25)		0.39 (20) [lq]	24.56	0.1147
Isopropyl formate 1-Isopropyl-4-	0.512 (20)	2.24 (20)	0	24.56 29.44 (20)	0.1147
methylbenzene	3.402 (20) 1.600 (30)	2.24 (20)	0	29.44 (20)	
Isoquinoline	3.253 (30)	10.7 (20)	2.75 [g]		
isoquinoinie	3.233 (30)	10.7 (20)	2.55 (25) [B]		
Lactamide					
Lactic acid	40.33 (25)	22 (17)			
Lactonitrile	2.01 (30)	38 (20)		38.31	0.0960
D-Limonene	2.01 (50)	2.4 (20)	1.57 (25) [B]	29.50	0.0929
DL-Limonene		2.3 (20)	0.63 (25) [B]	29.11	0.0913
DL-Mandelonitrile		17.8 (23)		45.90	0.0988
Menthol	6.89 (35)	17.0 (23)	1.55 (20) [B]	43.70	0.0700
2-Mercaptoethanol	3.4 (20)		1.55 (20) [2]		
Methacrylic acid	1.32 (20)		1.65	26.5 (25)	
Methacrylonitrile	0.392 (20)		3.69 [g]	24.4 (20)	
Methane [g]	0.010 9 (20)	1.000 94 (0)	0	*	
	0.013 3 (100)				
Methanesulfonic acid				52.28	0.0893

 $^{*\ 38.618\!-\!0.1873}T\!-\!0.000356T^2$

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

		5	D	Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Methanethiol Methanol	0.676 (10) 0.544 (25)	41.8 (-20) 33.62 (20)	1.26 [g] 1.69 [g] 1.68 (22) [B]	28.09 24.00	0.169 6 0.077 3
o-Methoxy- benzaldehyde	0.344 (23)	33.02 (20)	4.34 (20) [B]	45.34	0.1105
<i>p</i> -Methoxy- benzaldehyde		22.3 (22) 10.4 (248)	3.26 (35) [B]	44.69	0.1047
Methoxybenzene	1.152 (15) 0.789 (30)	4.33 (25) 3.9 (70)	1.36 [g] 1.24 (20) [B]	38.11	0.1204
2-Methoxyethanol	1.72 (20) 1.60 (25)	16.93 (25) 16.0 (30)	2.04 (25) [B]	33.30	0.098 4
2-(2-Methoxy- ethoxy)ethanol	3.48 (25) 1.61 (60)			34.8 (25)	29.9 (75)
2-Methoxyethyl acetate		8.25 (20)	2.13 (30) [B]		
1-Methoxy-2- nitrobenzene			4.83 [g]	48.62	0.1185
o-Methoxyphenol 2-Methoxy-4- (2-propenyl) phenol	6.931 (25)	12 (25)	2.46 (25) [B]	41.2	0.0943
o-Methoxytoluene m-Methoxytoluene		3.5 (20) 3.5 (20)			
<i>p</i> -Methoxytoluene <i>N</i> -Methyl- acetamide	3.88 (30) 2.54 (45)	4.0 (20) 178.9 (30) 138.6 (60)	4.39 (20) [D]	36.20 33.67 (30)	0.107 1 30.62 (50)
Methyl acetate	0.388 (20) 0.320 (40)	7.03 (20) 6.68 (25)	1.70 [g] 1.75 (25) [B]	27.95	0.1289
Methyl acetoacetate	1.704 (20)			34.98	0.0944
Methyl acrylate Methylamine	1.398 (20) 0.285 (15) 0.236 (0)	11.4 (-10)	1.77 (25) [B] 1.29 [g]	22.87	0.148 8
<i>N</i> -Methylaniline	2.02 (25) 1.084 (55)	10.0 (18)	1.67 (25) [B]	39.32	0.097 0
Methyl benzoate	2.298 (15) 1.673 (30)	6.59 (20)	1.86 (25) [B]	40.10	0.117 1
2-Methyl-1, 2-butadiene	0.266 (0.3) 0.223 (20)	2.1 (25)	0.15 [g]		
2-Methylbutane	0.237 (15) 0.215 (25)	1.871 (0) 1.845 (20)	0.13 [g]	17.20	0.1103
2-Methyl-1- butanol	5.50 (20) 1.44 (60)	14.7 (25)		21.5 (25)	
2-Methyl-2- butanol	5.48 (15) 2.81 (30)	5.82 (25)	1.72 (20) [B]	24.18	0.0748

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

		D. 1	D	Surface to dyn·c	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
3-Methyl-1- butanol	4.81 (15) 2.96 (30)	14.7 (25) 5.82 (130)	1.82 (25) [B]	25.76	0.0820
3-Methyl-2-butanol	3.51 (25)			23.0 (25)	
2-Methyl-1-butene		2.20 (20)	0.52 (20) [lq]	18.81	0.1148
2-Methyl-2-butene			0.11 (25) [lq] 0.34 (25) [B]	19.70	0.127 1
3-Methyl-1-butene		1.002 8 (100) [g]	0.25 [g]	16.42	0.103 1
2-Methylbutyl	0.872 (20)	4.63 (30)	1.82 (22)	26.75	0.0989
acetate Mathyl hydrigate	0.590 (20)	5.6 (20)	1.70 (22) [D]	27.48	0.1145
Methyl butyrate	0.580 (20) 0.459 (40)	5.6 (20)	1.72 (22) [B]	27.46	0.1143
3-Methylbutyric	2.731 (15)	2.64 (20)	0.63 (25)	27.28	0.0886
acid	2.411 (20)				
3-Methylbuty- ronitrile		18 (220)	3.62 (25) [C]	27.58	0.082 7
Methyl		12.9 (21)		37.90	0.1304
chloroacetate					
Methyl	3.82 (50) 2.69 (65)	19.23 (50)		41.32	0.107 4
cyanoacetate Methyl-	0.734 (20)	17.57 (65) 2.02 (20)	0	26.11	0.113 0
cyclohexane	0.734 (20)	2.07 (25)	O	20.11	0.1130
cis-2-Methyl-	18.08 (25)	13.3*	2.58 (30) [lq]*	32.45	0.077 0*
cyclohexanol	13.60 (30)		1.95 (25) [B]*		
trans-2-Methyl-	37.13 (25)				
cyclohexanol	25.14 (30)				
cis-3-Methyl-	19.7 (25)	16.47 (20)	1.91	29.08	0.062 9*
cyclohexanol	17.23 (30)				
trans-3-Methyl-	25.52 (16)	8.05	1.75	28.80 (30)	
cyclohexanol	15.60 (30)	12.2*	2.70 (20) [1.1*	20.07	0.060.0*
cis-4-Methyl- cyclohexanol	0.247 (25)	13.3*	2.70 (30) [lq]* 1.9 (25) [B]*	29.07	0.069 0*
trans-4-Methyl-	0.385 (25)		1.9 (23) [D]*		
cyclohexanol	0.363 (23)				
2-Methylcyclo-		16 (-15)	2.98 (25) [B]	34.06	0.1027
hexanone		14 (20)	2.50 (25) [B]	31.00	0.102 /
3-Methylcyclo-		18 (-80)	3.06 (25) [B]	33.06	0.0925
hexanone		12 (20)	, , , , ,		
4-Methylcyclo-		15 (-41)	3.07 (25) [B]	32.83	0.093 5
hexanone		12 (20)			
Methylcyclo-	0.507 (20)	1.985 (20)	0	24.63	0.1163
pentane	0.478 (25)		1 (5 (00) 517	20.22	0.001.2
Methyl decanoate			1.65 (20) [H]	30.33	0.091 2
Methyl dichloroacetate				37.00	0.121 9
dicinoroacetate					

^{*} Mixed isomers.

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Methyl			1.70 (20) [H]	31.37	0.089 3
dodecanoate N-Methyl-	1.99 (15)	200.1 (15)	3.86 (25) [B]	37.96 (30)	35.02 (50)
formamide Methyl formate	1.65 (25) 0.360 (15)	182.4 (25) 8.5 (20)	1.77 [g]	28.29	0.157 2
Methyl heptanoate 2-Methyl-2- heptanol 2-Methyl-3- heptanol 2-Methyl-4- heptanol 3-Methyl-3- heptanol 3-Methyl-4- heptanol 4-Methyl-3- heptanol 4-Methyl-4- heptanol	0.319 (29)	3.38 (-7) 2.46 (25) 3.37 (20) 3.75 (60) 3.30 (20) 3.65 (60) 3.74 (20) 2.89 (60) 9.1 (-20) 7.4 (20) 5.25 (20) 4.62 (55) 2.87 (20) 3.27 (60)	1.63 (20) [B]	28.29	0.157 2
Methyl hexadecanoate		3.27 (00)		31.50	0.077 5
2-Methylhexane 3-Methylhexane Methyl hexanoate Methyl isobutyrate	0.378 (20) 0.372 (20) 0.523 (20) 0.419 (40)	1.92 (20) 1.93 (20)	0 0 1.70 (20) [H] 1.98 (20) [B]	21.22 21.73 28.47 25.99	0.096 64 0.097 0 0.104 5 0.113 1
Methyl methacrylate	0.632 (20)	2.9 (20)	1.68 (25) [B]	28–29 (30)	
Methyl <i>o</i> -metho- xybenzoate Methyl <i>p</i> -metho-		7.7 (21) 4.3 (33)			
xybenzoate 1-Methylnaph-		2.7 (20)	0.23 (20) [B]	39.96	0.0934
thalene Methyl <i>o</i> -nitro- benzoate		28 (25)	3.67 (30) [B]		
Methyl octadecanoate				32.20	0.77 5
2-Methyloctane 4-Methyloctane Methyl octanoate		1.97 (20) 1.97 (20)	0 0	23.76 24.22 29.93	0.094 0 0.094 0 0.100 2
Methyl oleate 2-Methylpentane	4.88 (20) 0.310 (20) 0.295 (25)	3.211 (20) 1.88 (20)	0	31.3 (25) 19.37	25.4 (100) 0.099 7

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	ension
	V::	Dielectric	D:1-	dyn·c	
Substance	Viscosity η , mN·s·m ⁻²	constant, ε	Dipole moment, D	а	b
3-Methylpentane	0.307 (25) 0.292 (30)	1.895 (20)	0	20.26	0.1060
2-Methyl-2, 4-pentanediol	34.4 (20)		2.9 (0)	33.1 (20)	
4-Methylpen- tanenitrile	0.980 (20) 9.843 (30)	15.5 (22)	3.53 (25) [B]	28.89	0.0917
Methyl pentanoate 2-Methyl-1- pentanol	0.713 (20)	4.3 (19)	1.62 (22) [B]	27.85 26.98	0.104 4 0.081 9
3-Methyl-1- pentanol				26.92	0.0789
4-Methyl-1- pentanol				25.93	0.0743
2-Methyl-2- pentanol				25.07	0.086 1
3-Methyl-2- pentanol				27.14	0.0919
4-Methyl-2- pentanol	4.074 (25)			24.67	0.082 1
2-Methyl-3- pentanol				26.43	0.0914
3-Methyl-3-				25.48	0.0888
pentanol 4-Methyl-2-	0.585 (20)	13.11 (20)		23.64 (20)	19.62 (60)
pentanone 4-Methyl-3-	0.522 (30) 0.879 (25)	11.78 (40) 15.6 (0)	3.20 (25) [B]		
penten-2-one 1-Methyl-1-		15.1 (20) 7.3 (19)	1.84 (15) [B]		
phenylhy- drazine					
Methyl phenyl sulfide			1.38 (20) [B]	42.81	0.123 8
2-Methylpropane 2-Methylpro-	0.007 44 (20) [g] 0.551 (15)	20.2	0 4.07 [g]	12.83	0.123 6
panenitrile 2-Methyl-1- propanol	0.456 (30) 4.70 (15) 2.876 (30)	26 (-34) 17.93 (25)	3.60 (20) [B] 2.96 (30) [lq] 1.78 (20) [B]	24.53	0.079 5
2-Methyl-2- propanol	3.316 (20) 2.039 (40)	10.9 (30) 8.49 (50)	1.67 (22) [B]	20.02 (15)	19.10 (30)
2-Methylpropene			0.50 [g]	14.84	0.1319
N-Methylpro- pionamide	6.06 (20) 3.56 (40)	185 (20) 151 (40)	3.59 [g]	31.20 (20)	29.12 (50)
Methyl propionate 2-Methylpro-	0.477 (15) 1.213 (25)	6.21 2.73 (40)	1.70 (22) [B] 1.08 (25) [lq]	27.58 25.55 (20)	0.125 8 25.13 (25)
pionic acid	1.126 (30)				

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
1-Methylpropyl acetate				25.72	0.105 4
2-Methylpropyl acetate	0.702 (20) 0.366 (78)	5.29 (20)	1.87 (22) [B]	25.59	0.101 3
2-Methylpropy- lamine	21.7 (25)	4.43 (21)	1.27 (27)	24.48	0.109 2
2-Methylpropyl formate	0.680 (20)	6.41 (19)	1.88 (22)	26.14	0.1122
Methyl propyl ketoxime		3.3 (20)			
2-Methylpyridine	0.805 (20) 0.710 (30)	9.8 (20)	1.96 (25) [B]	36.11	0.1243
3-Methylpyridine			2.41 (25) [B]	37.35	0.1153
4-Methylpyridine			2.60 (25) [B]	37.71	0.114 1
N-Methyl-2- pyrrolidinone	1.666 (25)	32.0 (25)	4.09 (30) [B]		
Methyl salicylate		9.41 (30)	2.47 (25) [B]	42.15	0.1174
Methyl tetrade- canoate			1.62 (25) [B]	31.00	0.0800
2-Methyltetra- hydrofuran	0.601 (0) 0.536 (10)	6.92 (0) 6.63 (10)			
Methyl thiocyanate	64.3 (0)	4.3 (19)	3.34 (20) [B]	40.66	0.130 5
Morpholine	2.53 (15) 1.79 (30)	7.33 (25)	1.75 (25) [lq] 1.52 (25) [B]	37.63 (20)	36.24 (30)
Naphthalene	0.780 (100) 0.967 (80)	2.54 (85)	0	42.84	0.1107
1-Naphthonitrile		16 (70)			
2-Naphthonitrile		17 (70)			
o-Nitroaniline		34.5 (90)	4.28 (20) [B]		
<i>p</i> -Nitroaniline		56.3 (160)	6.3 (25) [B]	60.62	0.0923
o-Nitroanisole Nitrobenzene	2.165 (15)	24.92 (25)	4.83 [g]	48.62 46.34	0.118 5 0.115 7
Nitrobenzene	2.165 (15) 1.55 (35)	34.82 (25) 24.9 (90)	4.22 [g] 3.96 (25) [B]	40.34	0.115 /
<i>m</i> -Nitrobenzyl alcohol	1.55 (55)	24.9 (90)	3.90 (23) [В]		
2-Nitrobiphenyl	12 (45)		3.82 (20) [B]		
Nitroethane	0.677 (20)	28.06 (30)	3.61 [g]	35.27	0.125 5
	0.63 (35)	27.4 (35)			
Nitromethane	0.692 (15) 0.596 (30)	35.87 (30) 35.1 (35)	3.46 [g]	40.72	0.1678
1-Nitro-2- methoxy- benzene			4.83 [g]	48.62	0.118 5
o-Nitrophenol	2.343 (45)	17 (50)	3.14(25)[B]	47.35	0.1174
1-Nitropropane	0.798 (25) 0.70 (35)	23.24 (30) 22.7 (35)	3.60 [g]	32.62	0.1009

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
2-Nitropropane N-Nitrosodime- thylamine	0.750 (25)	25.52 (30) 53 (20)	3.76 [g] 4.01 (20) [B]	32.18	0.115 8
o-Nitrotoluene	2.37 (20) 1.63 (40)	27.4 (20) 22.0 (58)	3.72 (20) [B]	44.10	0.1174
<i>m</i> -Nitrotoluene	2.33 (20) 1.60 (40)	24 (20) 22 (58)	4.20 (20) [B]	43.54	0.1118
<i>p</i> -Nitrotoluene Nonane	1.20 (60) 0.713 (20) 0.666 (25)	22 (52) 1.972 (20) 1.85 (110)	4.47 (25) [B] 0	42.26 24.72	0.097 4 0.093 5
1-Nonanol 1-Nonene	14.3 (20) 0.620 (20) 0.586 (25)		1.72 (20) [B] 0.59 (20) [B]	29.79 24.90	0.078 9 0.093 8
(Z,Z)-9,12- Octadeca- dienoic acid		2.70 (70) 2.60 (120)	1.40 (18) [Hx]		
Octamethylcy- clotetrasiloxane	2.20 (20)	2.4 (20)	0.42 (25) [lq] 0.67 (25) [B]	20.19	0.081 1
Octamethyltri- siloxane	0.82 (20)	2.3 (20)	0.64 (25) [lq]	67.56 (25)	
Octane	0.546 (20) 0.433 (40)	1.95 (20) 1.83 (110)	0	23.52	0.095 1
Octanenitrile	1.811 (15) 1.356 (30)	13.90 (25)		29.61	0.080 2
Octanoic acid	5.828 (20) 4.690 (25)	2.45 (20)	1.15 (25) [lq]	29.2 (20)	28.7 (25)
1-Octanol	10.64 (15) 6.125 (30)	11.3 (10) 10.34 (20)	1.72 (20) [B]	29.09	0.079 5
2-Octanol		8.20 (20) 6.52 (40)	1.65 (20) [B]	27.96	0.0820
2-Octanone		10.39 (20) 7.42 (100)	2.72 (15) [B]		
1-Octene	0.470 (20) 0.447 (25)	2.084 (20)	0.34 (20) [lq]	23.68	0.095 8
Oleic acid	38.80 (20) 27.64 (25)	2.46 (20) 2.45 (60)	1.44 (25) [lq]	32.80 (20)	27.94 (90)
Oxalyl chloride 2-Oxohexame- thyleneimine	9 (78)	3.5 (21)	0.93 (20) [B] 3.88 (25) [B]		
4-Oxopentanoic acid				41.69	0.0763
Palmitic acid Paraldehyde Parathion	15.30 (25)	2.3 (70) 13.9 (25)	1.91 (25) [lq] 4.98 (25) [B]	28.28 39.2 (25)	0.1062

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	,
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Pentachloroethane	2.741 (15) 2.070 (30)	3.73 (20)	0.92 [g] 0.98 (25) [lq]	37.09	0.1178
Pentadecane	2.814 (22)		0	28.78	0.085 7
cis-1,3-Pentadiene		2.32 (25)	0.50 (25) [B]		
Pentanaldehyde		10.1 (17)	2.59 (20) [B]	27.96	0.1010
Pentane	0.237 (15)	2.011(-90)	0	18.25	0.1121
	0.215 (25)	1.84(20)			
1,5-Pentanediol	128 (20)	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	2.45 (20) [D]	43.2 (20)	
2,4-Pentanedione	0.6 (20)	25.7 (20)	3.03 [g]	33.28	0.1144
		17.39 (25)	2.5 (20) [B]		
Pentanenitrile	0.779 (15)	17.4 (21)	3.57 (25) [B]	27.44 (20)	26.33 (30)
	0.637 (30)				
1-Pentanethiol		4.55 (25) 4.23 (50)	1.54 (25) [lq]		
Pentanoic acid	2.359 (15)	2.66 (20)	1.61 (20) [D]	28.90	0.0887
i cintanoie acia	1.774 (30)	2.00 (20)	1.01 (20) [2]	20.70	0.000 /
1-Pentanol	4.650 (15)	16.9 (20)	1.71 (20) [B]	27.54	0.0874
	2.987 (20)	13.9 (25)	(==, [=]		
2-Pentanol	5.130 (15)	13.82 (22)	1.66 (22) [B]	25.96	0.1004
	2.780 (30)		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
3-Pentanol	7.337 (15)	13.02 (22)	1.64 (22) [B]	24.60 (20)	23.76 (30)
	3.306 (30)		, , , ,		
2-Pentanone	0.473 (25)	15.45 (20)	2.72 (22) [B]	24.89	0.065 5
		11.73 (80)			
3-Pentanone	0.493 (15)	19.4(-20)	2.72 (20) [B]	27.36	0.1047
	0.423 (30)	17.00 (20)			
1-Pentene	0.24(0)	2.10(20)	0.34 (20) [lq]	18.20	0.1099
cis-2-Pentene				19.73	0.1172
trans-2-Pentene				18.90	0.0997
Pentyl acetate	0.924 (20)	4.75 (20)	1.72 [g]	27.66	0.0994
	0.862 (25)		1.91 (25) [B]		
Pentylamine	1.018 (20)	4.5 (22)	1.55 (30) [B]	24.4 (13)	
Pentyl formate		6.5 (20)		28.09	0.1023
Pentyl nitrate		9 (18)			
Phenanthrene		2.8 (20)	0		
Phenol	6.024 (35) 3.421 (50)	9.78 (60)	1.53 (20) [B]	43.54	0.106 8
Phenoxyacetal- dehyde		4.8 (20)			
Phenoxyacetylene 2-Phenyl-		4.8 (20)	1.42 (25) [lq]	46.26	0.0788
acetamide					
Phenyl acetate	1.799 (45)	5.23 (20)	1.54 (22) [B]		
Phenylacetonitrile	1.93 (25)	19.0 (25) 8.5 (234)	3.47 (27) [B]	44.57	0.115 5

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface t	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Phenylacetylene		3.0 (20)	0.72 (20) [B]		
1-Phenylethanol		13 (20) 7.6 (90)	1.51 (20) [B]	42.88	0.103 8
Phenylhydrazine		7.2 (21)	1.67 (25) [B]	48.14	0.129 2
Phenyl isocyanate		8.8 (20)	1.07 (23) [B]	40.14	0.12) 2
Phenyl isothio- cyanate		10 (20)		42.73	0.108 6
1-Phenylpropene		2.7 (20)			
2-Phenylpropene		2.3 (20)			
3-Phenylpropene		2.6 (20)		24.27	0.105.6
Phenyl propyl ether				34.27	0.105 6
Phenyl salicylate		6.3 (50)		45.20	0.097 6
Phosgene		4.7 (0)			
		4.3 (22)			
Phthalide		36 (75)			
DL-α-Pinene	1.61 (25)	2.64 (25)	0.60 (25) [B]	28.35	0.094 4
L-β-Pinene	1.70 (20) 1.41 (25)	2.76 (20)		28.26	0.093 4
Piperidine	1.679 (15)	5.8 (20)	1.19 (25) [B]	31.79	0.115 3
1 iperiume	1.224 (30)	0.0 (20)	1115 (20) [25]	01	0.1100
Propane [g]	0.008 1 (20)	1.6(0)	0	9.22	0.087 4 [lq]
	0.0107 (125)				
1,2-Propane- diamine	1.46	10.2			
1,3-Propane- diamine	17.85	9.55	1.96 (25) [B]		
1,2-Propanediol	56.0 (20)	32.0 (20)	2.27 (25) [D]	72.0 (25)	
1.2 Duamanadial	18.0 (40)	25.0 (20)	2.52 (25) [D]	47.43	0.000.2
1,3-Propanediol	56.0 (20) 18.0 (40)	35.0 (20)	2.52 (25) [D]	47.43	0.090 3
1-Propanethiol	10.0 (10)		1.55 (25) [lq]	27.38	0.127 2
2-Propanethiol			1.64 (25) [lq]	24.26	0.1174
1-Propanol	2.522 (15)	22.2 (20)	1.67 [g]	25.26	0.077 7
	1.722 (30)	20.33 (25)	1.75 (25) [B]		
2-Propanol	2.859 (15)	18.3 (25)	1.69 [g]	22.90	0.078 9
2 D 11 1 1	1.765 (30)	16.24 (40)	1.66 (30) [B]		
2-Propenaldehyde			3.04 [g]		
Propene [g]	0.008 43 (20)	1.88 (20)	2.90 (25) [B] 0.35 [g]	9.99	0.142 7 [lq]
r ropene [g]	0.009 33 (50)	1.44 (90)	0.55 [6]	7.77	0.1 12 / [iqj
2-Propen-1-ol	1.363 (20)	21.6 (15)	1.63 [g]	27.53	0.0902
•	0.914 (40)	, ,			
Propionaldehyde	0.357 (15)	18.5 (17)	2.75 [g]		
	0.317 (27)		2.57 (20) [B]		

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Propionamide			3.4 (30) [B]	39.05	0.0909
Propionic acid	1.175 (15)	3.30(10)	1.76 [g]	28.68	0.0993
•	0.956 (30)	3.44 (40)	1.77 (25) [D]		
Propionic	1.144 (20)	18.3 (16)		30.30 (20)	29.70 (25)
anhydride	1.061 (25)				
Propionitrile	0.454 (15)	22.2 (20)	4.06 [g]	29.63	0.1153
•	0.389 (30)	24.2 (50)	3.60 (20) [B]		
Propyl acetate	0.585 (20)	5.69 (19)	1.86 (25) [B]	26.60	0.1120
	0.460 (40)				
Propylamine	0.343 (25)	5.31 (20)	1.17 [g]	24.86	0.1243
			1.36 (20) [B]		
Propylbenzene		2.37 (20)	0.35 (25) [lq]	31.13	0.107 5
		2.351 (30)			
Propyl benzoate				36.55	0.1069
Propyl butyrate	0.831 (20)	4.3 (20)		27.06	0.1000
Propyl				32.91	0.1083
chloroacetate					
Propylene	2.53	64.4			
carbonate					
Propylene oxide	0.327 (20)		2.00 [g]		
	0.28 (25)				
Propyleneimine	0.491 (25)		1.77 [g, cis]		
			1.60 [g, trans]		
Propyl formate	0.574 (20)	7.72 (19)	1.91 (22) [B]	26.77	0.1119
	0.417 (40)				
Propyl isobutyrate	0.831 (20)			25.83	0.1015
Propyl nitrate		14 (18)	3.01 (20) [B]	29.67	0.123 7
Propyl pentoate	1.053 (20)	4(19)		27.72	0.0984
Propyl propionate	0.673 (20)	4.7 (20)	1.79 (22) [B]	26.85	0.105 9
Propyne			0.75 [g]	14.51	0.148 2
2-Propyn-1-ol	1.68 (20)	24.5 (20)	1.78 (25) [B]	38.59	0.127 0
Pulegone		9.5 (20)	2.00 (25) [B]		
Pyradazine			3.97 (35) [D]	50.55	0.103 6
Pyrazine		2.8 (54)	0		
Pyridine	1.130 (10)	12.3 (25)	2.20 (20) [B]	39.82	0.1306
	0.829 (30)	9.4 (116)	2.25 [g]		
Pyrimidine			2.44 (35) [D]	32.85	0.1010
Pyrrole	1.352 (20)	7.48 (18)	1.80 (25) [B]	39.81	0.1100
	1.233 (25)	8.13 (25)			
Pyrrolidine			1.58 (20) [B]	31.48	0.0900
2-Pyrrolidone	13.3 (25)		3.55 (25) [B]		
Quinoline	4.354 (15)	9.00 (25)	2.18 (25) [B]	45.25	0.1063
Ç	3.37 (25)	/	(,[-]		
Safrole	2.294 (25)	3.1 (21)			
	1 '	1 ' '	2 1 (20) [[-7]	45.38	0.1242
Salicylaldehyde	2.90 (20)	13.9 (20)	3.1 (30) [lq]	43.38	U.124 Z
	1.67 (45)		2.86 (20) [B]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	,
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Squalane Squalene	6.08 (20) 12 (25)		0 0.68 (25) [B]		
D-Sorbitol		33 (80)			
Stearic acid	11.6 (70)	2.29 (70) 2.26 (100)	1.76 (25) [D]		
Styrene	0.751 (20) 0.696 (25)	2.43 (25) 2.32 (75)	0.13 (25) [lq]	32.0 (20)	30.98 (30)
Succinonitrile	2.591 (60) 2.008 (75)	56.5 (57) 54 (68)	3.68 (30) [toluene]	53.26	0.107 9
1, 1,2,2-	13.950 (11)	8.6(3)	1.29 (20) [H]	52.37	0.1463
Tetrabromo- ethane	9.797 (20)	7.0 (22)			
1, 1,2,2-	1.21 (25)	2.52 (25)		26.13	0.1133
Tetrachloro- difluoroethane	1.208 (30)				
1, 1,2,2-Tetrach- loroethane	1.844 (15) 1.456 (30)	8.20 (20)	1.29 [g] 1.45 (25) [H]	38.75	0.1268
Tetrachloro- ethylene	1.932 (15) 0.798 (30)	2.30 (25)	0	32.86 (15)	31.27 (30)
Tetradecamethyl- cyclohepta- siloxane	0.798 (30)	2.7 (20)			
Tetradecamethyl- hexasiloxane		2.5 (20)	1.58 (20) [lq]	17.42 (25)	
Tetradecane	2.131 (22)		0	28.30	0.0869
Tetradecanoic acid		0.76 (25) [B]	33.90	0.093 2	
1-Tetradecanol		4.72 (38) 4.40 (48)	1.69 (25) [C]	32.72	0.0703
Tetraethylene glycol	44.9 (25)		5.84 (20) [lq]	45 (25)	
Tetraethyllead			0.3 (20) [B]	30.50	0.0969
Tetraethylsilane			0	25.22	0.1079
Tetraethyl silicate		4.1 (20)	1.72 (32) [B]	23.63	0.0979
Tetrahydrofuran	0.55 (20)	11.6 (-70)	1.75 (25) [B]	26.5 (25)	
2,5-Tetrahydro-	0.460 (25) 225 (25)	7.58 (25)			
furandi- methanol	223 (23)				
Tetrahydro-2- furanmethanol	6.24 (20)	13.61 (23)	2.12 (35) [lq]	39.96	0.1008
1,2,3,4-Tetrahy- dronaphthalene	2.202 (20) 2.003 (25)	2.76 (20)	0.60 (25) [lq]	35.55	0.0954
1,2,3,4-	(20)	11.7 (20)			
Tetrahydro- 2-naphthol		6.7 (90)			

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	,
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Tetrahydropyran	0.826 (20) 0.764 (25)	5.61 (25)	1.55 (25) [B]		
Tetrahydropyran- 2-methanol	11.0 (20)			34.1 (25)	
Tetrahydrothi- ophene-1, 1-dioxide	9.87 (30)	43.3 (30)	4.81 (25) [B]	35.5 (30)	
Tetrahydrothio- phene oxide	52 (30) 19 (80)	42.5 (30)			
1,1,2,2-Tetra- methylurea		23.06	3.47 (25) [B]		
Tetranitromethane Tetrathiomethyl- methane	1.76 (20)	2.32 (20) 2.82 (70)	0		
Thiacyclohexane Thiacyclopentane	1.042 (20) 0.971 (25)		1.90 (25) [B]	36.06 (20) 38.44	33.74 (40) 0.134 2
Thioacetic acid		12.8 (20)			
2,2'-Thiodiethanol Thiophene	65.2 (20) 0.662 (20) 0.353 (82)	2.76 (16) 2.57 (25)	0.55 [g] 0.52 (25) [B]	53.8 (20) 34.00	0.1328
Thymol	0.333 (82)	2.37 (23)	1.55 (25) [B]	33.95	0.082 1
Toluene	0.623 (15) 0.523 (30)	2.385 (20) 2.364 (30)	0.45 (20) [lq]	30.90	0.1189
<i>p</i> -Toluenesulfonyl chloride				42.41	0.0903
o-Toluidine	5.195 (15) 4.39 (20)	6.34 (18) 5.71 (58)	1.60 (25) [B]	42.87	0.1094
<i>m</i> -Toluidine	4.418 (15) 2.741 (30)	5.95 (18) 5.45 (58)	1.45 (25) [B]	40.33	0.0979
<i>p</i> -Toluidine	1.945 (45) 1.557 (60)	4.98 (54)	1.52 (25) [B]	39.58	0.095 7
<i>m</i> -Tolunitrile			4.21 (22) [B]	38.85	0.1013
<i>p</i> -Tolunitrile			4.47 (20) [B]	39.79	0.1100
Tribenzylamine Tributyl phosphite	1.9 (25)		0.65 (20) [B] 1.92 (20) [C]	42.41 27.57	0.095 3 0.086 5
2,2,2-Tribromo- acetaldehyde		7.6 (20)	1.70 (20) [B]		
Tribromoethane	2.152 (15) 1.741 (30)	4.39 (20)	0.99 [g]	48.14	0.1308
1,2,3-Tribro- mopropane		6.45 (20)	1.59 (25) [B]	47.99	0.1267
Tributylamine Tributyl borate	1.35 (25) 1.776 (20) 1.601 (25)		0.78 (25) [B] 0.78 (25) [C]	26.47 26.2 (20)	0.083 1 25.8 (25)

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Tributyl phosphate	111.1 (15)	3.39 (25)	7.96 (30) [B]	3.07 (25) 28.71	0.0666
Trichloroace- taldehyde		7.6 (-40) 4.9 (20)	1.96 (25) [B]	27.66	9.1197
Trichloroacetic acid		4.6 (60)	1.1 (25) [B, dimer]	35.4	0.089 5
Trichloro- acetonitrile		7.85 (19)	1.93 (19) [lq]		
1,1,1-Trichlo- roethane	0.903 (15) 0.725 (30)	7.1 (7) 7.52 (20)	1.79 [g] 1.6 (25) [B]	28.28	0.1242
1,1,2-Trichlo- roethane	0.119 (20) 0.110 (25)	8.78 (23)	1.45 [g]	37.40	0.135 1
Trichloroethylene	0.566 (20) 0.532 (25)	3.42 (16)	0.77 (30) [lq] 0.95 (30) [B]	29.5 (20)	28.8 (25)
Trichlorofluoro- methane	0.42 (25) 0.011 (25) [g]	2.28 (29)	0.45 [g] 0.49 [lq]	18 (25)	
Trichloro- methylsilane	0.47 (20)		1.87 (25) [B]	20.3 (20)	
2,4,6-Trichloro- phenol			1.88 (25) [D]	43.13	0.095 5
1,2,3-Trichloro- propane		7.5 (20)	1.61 [g]	37.8 (20)	37.05 (25)
Trichlorosilane	0.332 (20) 0.316 (25)		0.86 [g] 0.98 (25) [B]	20.43	0.107 6
α, α, α -Trichloro- toluene	3.07 (10) 2.55 (17)	6.9 (21)	2.17 (20) [B]		
1,1,2-Trichloro- 1,2,2,-trifluoro- ethane	0.711 (20) 0.627 (30)	2.41 (25)		17.75 (20)	16.56 (30)
Tridecane	1.883 (20) 1.55 (23)		0	27.73	0.087 2
1-Tridecene Triethanolamine	613.6 (25) 208.1 (40)	29.36 (25)	3.57 (25) [B]	28.01	0.0884
Triethylaluminum Triethylamine	0.394 (15)	2.9 (20) 2.42 (25)	0.66 [2]	22.70	0.099 2
	0.363 (30)		0.66 [g] 0.9 (25) [B]		
Triethylene glycol	49.0 (20) 8.5 (60)	23.7 (20)	5.58 (20) [lq]	47.33	0.088 0
Triethyl phosphate	1.684 (40) 1.376 (55)	13.43 (15) 10.93 (65)	3.08 (25) [B]	31.81	0.092 8
Triethyl phosphite	0.72 (25)	5.0	1.82 (25) [D]	25.73	0.0878

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TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

				Surface to	
Substance	Viscosity η , mN·s·m ⁻²	Dielectric constant, ε	Dipole moment, D	а	b
Trifluoroacetic acid	0.926 (20) 0.653 (40)	8.55 (20) 5.76 (50)	2.28 [g]	15.64	0.1844
2,2,2-Trifluoro- ethanol	1.996 (20)	3.70 (30)	2.03 (25) [cH]	20.6 (33)	
α, α, α -Trifluoro- toluene		9.2 (30) 8.1 (60)			
Trimethylamine 1,2,3-Trimethylbenzene	0.321 (-33)	2.4 (25) 2.636 (20) 2.609 (30)	0.56 (20) [lq]	16.24 30.91	0.113 3 0.104 0
1,2,4-Trimethyl- benzene	0.894 (15) 0.730 (30)	2.38 (20) 2.36 (30)	0.30 (20) [lq]	31.76	0.1025
1,3,5-Trimethyl- benzene	1.154 (20)	2.28	0	29.79	0.0897
Trimethyl borate 2,2,3-Trimethyl-butane	0.579 (20)	8 (20) 1.93 (20)	0.82 (25) [C] 0	20.70	0.0973
cis, cis-1,3,5- Trimethyl- cyclohexane trans-1,3,5-	0.632 (20) 0.558 (30)				
Trimethyl-cyclohexane Trimethylene sulfide 3,5,5-Trimethyl- 1-hexanol	0.714 (20) 0.624 (30) 0.638 (20) 0.607 (25) 11.06 (25)		1.78 (25) [B]	36.3 (20)	35.0 (30)
2,6,8-Trimethyl- 4-nonanone	1.9 (20)				
1,3,5-Trimethyl- 2-oxabicyclo-		4.57 (24)	1.54 (25) [C]	32.1 (20)	31.1 (25)
[2.2.2]octane 2,2,3-Trimethyl- pentane	0.598 (20)	1.962 (20)	0	22.46	0.089 5
2,2,4-Trimethyl- pentane	0.502 (20)	1.940 (20)	0	20.55	0.0888
Trimethyl phosphite	0.61 (20)		1.83 (20) [C]	27.18 (20)	24.88 (40)
2,4,6-Trimethyl- pyridine	1.498 (20) 1.496 (25)	6.6	1.95 (25) [B]		
Triphenylamine Triphenyl	25.18 (15)	3.67 (45)	2.04 (25) [B]	46.2	0.095 5
phosphite Tripropylamine	6.95 (45)	3.57 (65)	0.58 (20) [lq] 0.76 (20) [B]	24.58	0.087 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

		5.1	D. 1	Surface to	
Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	а	b
Tripropylene glycol	56.1 (25)			34 (25)	
Tripropylene glycol butyl ether	6.58 (25)			28.8 (25)	
Tripropylene glycol ethyl ether	5.17 (25)			28.2 (25)	
Tripropylene glycol isopropyl ether	7.7 (25)			27.4 (25)	
Tripropylene glycol methyl ether	5.96 (25)			30.0 (25)	
Tris(dimethy- lamino) phos- phine oxide	3.34 (30)	30 (20)			
Tris(4-ethyl- phenyl) phosphite	30.22 (15) 9.047 (45)	3.74 (15) 3.61 (45)	2.08 (25) [B]		
Tris(<i>m</i> -tolyl) phosphite	37.55 (15) 9.132 (45)	3.67 (15) 3.53 (45)	1.62 (25) [B]		
Tris(<i>p</i> -tolyl) phosphite	35.52 (15) 8.794 (45)	3.88 (15) 3.74 (45)	1.77 (25) [B]		
Tritolyl phosphate	38.8 (35) 16.8 (55)	6.92 (40)	2.84 (40) [C]	40.9 (20)	
Undecane	1.186 (20) 0.761 (50)	2.00 (20) 1.84 (150)	0	26.26	0.090 1
2-Undecanone Urea	1.61 (30)		2.71 (15) [B] 4.59 (25) [D]		
Vinyl acetate	0.421 (20)		1.79 (25) [B]	23.95 (20)	22.54 (30)
o-Xylene	0.809 (20) 0.627 (40)	2.57 (20) 2.54 (30)	0.62 [g] 0.52 (25) [lq]	32.51	0.110 1
m-Xylene	0.617 (20) 0.497 (40)	2.37 (20) 2.35 (30)	0.33 (20) [lq] 0.37 (20) [B]	31.23	0.1104
<i>p</i> -Xylene	0.644 (20) 0.513 (40)	2.26 (20) 2.22 (50)	0	30.69	0.107 4
Xylitol		40 (20)			

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TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substance

Temperature in degree celsius are indicated in parentheses. The physical state of the substance is indicated in square brackets

brackets					
	T	D. I.	Dipole	Surface te dyn·cr	
Substance	Viscosity, mN·s·m ⁻²	Dielectric constant, ε	moment,	а	b
Air (20°C) AlBr ₃	0.018 2	1.000 536 4 3.38 ¹⁰⁰	5.2		
Ar					
[g] (20°C)	0.022 3	1.000 517 2		24.20	0.240.2
[lq]		$1.538^{-191} \\ 8.83^{35}$	0	34.28	0.249 3
AsBr ₃		12.6^{20}	1.61 1.59	54.51 41.67	0.1043 0.097 81
AsCl ₃ AsH ₃ (arsine)		2.05^{20}	0.20	41.07	0.09/81
BBr ₃ (arsine)		2.58°	0.20	31.90	0.128 0
BCl ₃		2.36	0	31.70	0.1200
BF ₃			0	-2.92	0.2300
B_2H_6 (diborane)		$1.872^{-92.5}$	0	-3.13	0.178 5
B_5H_9			2.13		
B ₃ H ₆ N ₃ (triborotriazine)			0		
Br_2					
$[g](20^{\circ}C)$		1.0128			
[lq]	1.0316	3.09^{20}	0	45.5	0.182 0
BrF ₃	2.22^{20}		1.1	38.30	0.099 9
BrF ₅	0.62^{24}	$7.91^{24.5}$	1.51	25.24	0.109 8
Cl ₂					
[g] (20°C)	0.013 2		0		
[lq]	0.4012	1.9114	0.554	26.0	0.166.0
CIF ₃	0.4812	4.29^{25}	0.554 0.023	26.9 12.24	0.166 0 0.157 6
ClO ₃ F (perchloryl fluoride)			0.023	12.24	0.1370
Co					
[g]	0.0175^{20}	1.00070°	0.112		
[lq]	0.0173	1.000 70	0.112	-30.20	0.207 3
CO ₂				30.20	0.2073
[g] (20°C)	0.0147	1.000 922	0		
[lq]	0.071^{20}	1.60 ^{0 °C, 50 atm}			
COCl ₂		4.34^{22}	1.17	22.59	0.145 6
COF ₂			0.95		
COS			0.712	12.12	0.177 9
COSe		3.4710	0.73		
CS			1.98		
CS_2					
[g]	0.27520	1.0029^{0}	0		
[lq]	0.375^{20}	2.6^{20}	0.47		
CrO ₂ Cl ₂ [chromyl(VI)		2.6^{20}	0.47		
chloride] D ₂ (deuterium)		1.277^{-253}			
D ₂ (deuterium)		1.4//		6.537	0.188 3
D_2O	1.098 ²⁵	78.25 ²⁵	1.87	$(71.72^{20})*$	(68.38 ⁴⁰)*
D ₂ O	1.070	70.23	1.07	(11.12)	(00.50)

^{*}Actual values of surface tension.

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

		Did	Dipole	Surface tension, dyn·cm ⁻¹	
Substance	Viscosity, mN⋅s⋅m ⁻²	Dielectric constant, ε	moment,	а	b
F_2		1.54^{-202}		-16.10	0.1646
GaCl ₃			0.85	35.0	0.1000
GeCl ₄		2.430^{25}	0	$(22.44^{30})*$	
H_2					
$[g](20^{\circ}C)$	0.008 8	1.000 253 8	0		
[lq]		$1.228^{20.4 \text{ K}}$			
HBr					
[g]	0.02-67	1.003 130	0.82	12.10	0.207.0
[lq]	0.83^{-67}	3.82^{25}		13.10	0.207 9
HCl		1.004.60	1.00		
[g]	0.51^{-95}	$1.004 6^{0}$ 4.60^{28}	1.08		
[lq] HCN	0.31 0.206^{18}	116^{20}	2.98	(19.4510)*	(18.33 ²⁰)*
HCNO (isocyanate)	0.200	110	1.6	(19.45)	(10.33)
HCNS (isothiocyanate)			1.7		
HF	0.256°	83.6°	1.82	10.41	0.078 67
HI	0.230	05.0	1.02	10.11	0.07007
[g]		$1.002\ 34^{\circ}$	0.44		
[lq]		2.90^{22}			
NH ₃ (azide)			0.8		
H ₂ O (see Table 4.12)					
H_2O_2	1.25^{20}	84.2°	2.2	78.97	0.1549
HNO ₃			2.17		
H_2S					
[g]		1.00 ± 0^{0}	0.97		
[lq]	0.412^{0}	5.93^{10}		48.95	0.175 8
H ₂ Se	2 1 7 125	10025	0.24	22.32	0.148 2
H ₂ SO ₄	24.54 ²⁵	100^{25} 60^{20}			
HSO ₃ Cl (chlorosulfonic	2.43^{20}	60-0			
acid) HSO ₂ F (fluorosulfonic	1.56^{25}	$\sim 120^{25}$			
acid	1.30	~120			
H ₂ Te			< 0.2	29.03	0.2619
He			\ 0.2	27.03	0.201)
[g] (20°C)	0.0196	1.000 065 0	0		
Hg	1.552^{20}	1.000 000 0	0	490.6	0.2049
I_2	1.98 ¹¹⁶	11.1^{118}	0	., .,	
IF ₅			2.18	33.16	0.1318
Kr					
[g] (20°C)	0.025 0		< 0.05		
[lq]				40.576	0.2890
Ne[g] (20°C)	0.0313	1.000 063 9	0		
N_2					
[g] (20°C)	0.0176	1.000 548 0	0		
[lq]		1.454^{-203}		26.42	0.2265

^{*}Actual values of surface tension.

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TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

	3 7'	D' L . C	Dipole	Surface te dyn·cn	
Substance	Viscosity, mN⋅s⋅m ⁻²	Dielectric constant, ε	moment, D	а	b
NH ₃					
[g]	0.254-335	$1.007 2^{0}$	1.47	(27.01-50)*	(25 20-40)*
[lq]	$0.254^{-33.5}$ 0.97^{20}	$22.4^{-33.4} 52.9^{20}$	1.75	(37.91 ⁻⁵⁰)*	$(35.38^{-40})*$
N ₂ H ₄ (hydrazine) NO	0.97	32.9	0.153	-67.48	0.585 3
N ₂ O			0.133	-07.46	0.363 3
[g]	$0.014 6^{20}$	$1.001\ 13^{\scriptscriptstyle 0}$	0.167		
[lq]	0.0110	1.5215	0.107	5.09	0.203 2
NO ₂		1.52	0.316	3.07	0.203 2
N_2O_4		2.56^{15}	0.5		
NOBr (nitrosyl					
bromide)		13.4^{15}	1.8		
NOCI		18.2^{12}	1.9	29.49	0.1493
NOF			1.81	14.00	0.1165
NO ₂ F (nitryl fluoride)			0.47	8.26	0.1854
O ₂					
[g] (20°C)	0.0204	1.000 494 7	0		
[lq]		1.507^{-193}		-33.72	0.256 1
O_3			0.53	$(38.1^{-183})*$	
OF ₂ (oxygen difluoride)			0.297		
OsO ₄		***	0		
PBr ₃		3.9^{20}	0.5	45.34	0.128 3
PCl ₃		3.43^{25}	0.78	31.14	0.1266
PCl ₅		2.7^{165}	0.9		
PF ₅		0.015	0		
PH ₃		2.9 ¹⁵	0.58	(1.66	0.065.51
PI ₃	1.06525	4.12 ⁶⁵	0	61.66	0.067 71
POCl ₃	1.065^{25}	13.7^{25}	2.41	35.22	0.127 5
POF ₃		5.8^{22}	1.76 1.42	27.00	0.127 2
PSCl ₃ PbCl ₄		2.78^{20}	1.42	37.00	0.1272
S ₂ Cl ₂ dimer		4.79 ¹⁵	1.0	46.23	0.1464
S ₂ F ₂		4.79	1.0	40.23	0.1404
FSSF isomer			1.45		
S=SF ₂ isomer			1.03		
SF ₄			0.632	12.87	0.173 4
SF ₆			0	5.66	0.1190
S_2F_{10}		2.020^{20}	0		
SO ₂					
[g]	0.0126^{29}	$1.009~3^{\circ}$	1.63		
[lq]		15.0°		26.58	0.1948
SO ₃		3.11^{18}	0		
SOBr ₂ (thionyl bromide)		9.06^{20}	9.11		
		9.25^{20}	1.45	36.10	0.1416

^{*}Actual values of surface tension.

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

	7 7.	D: 1	Dipole	Surface te dyn·cn	
Substance	Viscosity, mN·s·m ⁻²	Dielectric constant, ε	moment, D	а	b
SO ₂ Cl ₂ (sulfuryl chloride)		9.15 ²⁰	1.81	32.10	0.1328
SbCl ₃ SbCl ₅		33.275 3.2220	3.93	47.87	0.123 8
SbF ₅ SbH ₃		3.22	0.12	49.07	0.1937
SeF ₄ SeF ₆			0.12	38.61	0.127 4
SeOCl ₂ SiCl ₄		55^{25} 2.40^{16}	2.64	20.78	0.099 62
SiF ₄ SiH ₄		2.10	0	20.70	0.055 02
SiHCl ₃ SnBr ₄			0.86	20.43	0.107 6
SnCl ₄ TeF ₆		2.89 ²⁰	0	29.92	0.1134
TiCl ₄ UF ₆		2.80^{20}	0	(33.54 ²⁰)*	(31.06 ⁴⁰)*
[g] [lq]		1.002 92 ⁶⁷ 2.18 ⁶⁵	0	25.5	0.1240
VCl ₄ VOBr ₃		3.05^{25} 3.6^{25}	0	23.3	0.1270
VOCl ₃ Xe [g] (20°C)	0.022 8	3.4 ²⁵ 1.001 23	0.3	(36.36 ²⁰)*	(33.60 ⁴⁰)*

^{*}Actual values of surface tension.

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TABLE 4.12 Refractive Index, Viscosity, Dielectric Constant, and Surface Tension of Water at Various Temperatures

Temperature, °C	Refractive index, $n_{\scriptscriptstyle D}$	Viscosity, mn·s·m ⁻²	Dielectric constant, ε	Surface tension, dyn·cm ⁻¹
0	1.333 95	1.770 2	87.74	75.83
5	1.333 88	1.5108	85.76	75.09
10	1.333 69	1.303 9	83.83	74.36
15	1.333 39	1.137 4	81.95	73.62
20	1.333 00	1.001 9	80.10	72.88
21	1.332 90	0.9764	79.73	72.73
22	1.332 80	0.953 2	79.38	72.58
23	1.332 71	0.931 0	79.02	72.43
24	1.332 61	0.9100	78.65	72.29
25	1.332 50	0.8903	78.30	72.14
26	1.332 40	0.8703	77.94	71.99
27	1.332 29	0.851 2	77.60	71.84
28	1.332 17	0.8328	77.24	71.69
29	1.332 06	0.8145	76.90	71.55
30	1.331 94	0.797 3	76.55	71.40
35	1.331 31	0.7190	74.83	70.66
40	1.330 61	0.6526	73.15	69.92
45	1.329 85	0.597 2	71.51	69.18
50	1.329 04	0.5468	69.91	68.45
55	1.328 17	0.504 2	68.35	67.71
60	1.327 25	0.4669	66.82	66.97
65	1.326 16	0.434 1	65.32	66.23
70	1.325 11	0.405 0	63.86	65.49
75	1.323 99	0.379 2	62.43	64.75
80		0.3560	61.03	64.01
85		0.335 2	59.66	63.28
90		0.3165	58.32	62.54
95		0.299 5	57.01	61.80
100		0.284 0	55.72	61.80

COMBUSTIBLE MIXTURES

TABLE 4.13 Properties of Combustible Mixtures in Air

Additional compounds can be found in National Fire Protection Association, *Fire Protection Handbood*, 14th ed., 1976.

	Audalianidian	Flammable limits, volume of f (25°C, 760 r	uel
Substance	Autoignition temperature, °C	Lower	Upper
Acetaldehyde	175	4.0	6.0
Acetic acid, glacial	465	5.4	16.0
Acetic anhydride	390	2.9	10.3
Acetone	465	2.6	12.8
Acetonitrile	524	4.4	16.0
Acetylene	305	2.5	100
Acrolein	235*	2.8	31.0
Acrylonitrile	481	3.0	17
Allyl alcohol	378	2.5	18.0
Allylamine	374	2.2	22
Ammonia, anhydrous	651	16	25
Aniline	615	1.3	
Benzene	560	1.3	7.1
Biscyclohexyl	245	0.7 (100°C)	5.1 (150°C)
1-Bromobutane	265	2.6 (100°C)	6.6 (100°C)
3-Bromopropene	295	4.4	7.3
Butane	405	1.9	8.5
Butanol	365	1.4	11.2
2-Butanone	516	1.8	10
1-Butene	385	1.6	10.0
3-Buten-1-ol		4.7	34
Butyl acetate	425	1.7	7.6
Butylamine	312	1.7	9.8
Butylbenzene	410	0.8	5.8
Butylene oxide		1.5	18.3
Butyl formate	322	1.7	8.2
Butyraldehyde	230	2.5	12.5
Butyric acid	450	2.0	10.0
Carbon disulfide	90	1.3	50.0
Carbon monoxide	609	12.5	74
Carbonyl sulfide		12	29
Chlorobenzene	640	1.3	7.1
2-Chloro-1,3-butadiene		4.0	20.0
1-Chlorobutane		1.8	10.1
2-Chloro-2-butene		2.3	9.3
1-Chloro-1,1-difluoroethane		6.2	17.9
2-Chloroethanol	425	4.9	15.9
Chloromethane	632	10.7	17.4

^{*}Unstable.

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TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

		Flammable limits, percent by volume of fuel (25°C, 760 mm)		
Substance	Autoignition temperature, °C	Lower	Upper	
1-Chloropentane	260	1.6	8.6	
2-Chloropropane	593	2.8	10.7	
1-Chloro-1-propene		4.5	16	
3-Chloro-1-propene	485	2.9	11.1	
Chlorotrifluoroethylene		8.4	38.7	
Crotonaldehyde	232	2.1	15.5	
Cumene	425	0.9	6.5	
Cyanogen	423	6.6	42.6	
Cyclohexane	245	1.3	8	
Cyclopropane	500	2.4	10.4	
yeloptopane	300	2.4	10.4	
Decahydronaphthalene	250	0.7	4.9	
Decane	210	0.8	5.4	
Diborane	38-52†	0.8	88	
Dibutyl ether	194	1.5	7.6	
o-Dichlorobenzene	648	2.2	9.2	
,2-Dichloroethylene		9.7	12.8	
Dichloropropane	557	3.4	14.5	
Diisopropyl ether	443	1.4	7.9	
Diethylamine	312	1.8	10.1	
Diethyl ether	160	1.9	36.0	
2,2-Dimethylbutane	425	1.2	7.0	
Dimethyl ether	423	3.4	27.0	
	445	1.2	7.0	
V,N-Dimethylformamide		2		
,1-Dimethylhydrazine	249		95	
2,3-Dimethylpentane	335	1.1	6.7	
2,2-Dimethylpropane	450	1.4	7.5	
Dimethyl sulfide	206	2.2	19.7	
Dimethyl sulfoxide	215	2.6	28.5	
,4-Dioxane	180	2.0	22.0	
Divinyl ether	360	1.7	27	
Ethane	515	3.0	12.5	
Ethanol	365	3.3	19	
2-Ethoxyethanol	235	1.8	14.0	
-Ethoxyethanol -Ethoxypropane	433	1.7	9.0	
	427	2.2	1	
Ethyl acetate	427		11.0	
Ethylamine	385	3.5	14.0	
Ethylbenzene	432	1.0	6.7	
Ethylcyclobutane	210	1.2	7.7	
Ethylene	490	2.7	36.0	
Ethyleneimine	320	3.6	46	
Ethylene oxide	429	3.6	100	
Ethyl formate	455	2.8	16.0	
,3-Ethylidene dichloride	440	6.2	16	
Ethyl nitrite	90	3.0	50	

 $^{^{\}dagger}\text{Ignites}$ in moist air.

TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

		Flammable limits, percent by volume of fuel (25°C, 760mm)		
Substance	Autoignition temperature, °C	Lower	Upper	
Ethyl propionate Ethyl vinyl ether	440 202	1.9 1.7	11 28	
Formaldehyde 2-Furaldehyde Furan Furfuryl alcohol	429 316 491	7.0 2.1 2.3 1.8	73 19.3 14.3 16.3	
Gasoline, 92 octane	~280	1.4	7.6	
Heptane Hexane 2-Hexanone Hydrocyanic acid, 96% Hydrogen 4-Hydroxy-4-methyl-2- pentanone	215 225 533 538 400 603	1.0 1.1 1.2 5.6 4.0 1.8	6.7 7.5 8 40.0 75 6.9	
Isobutyl acetate Isobutylbenzene Isopentane Isopentyl acetate Isoprene Isopropyl acetate Isopropyl alcohol	421 430 420 360 220 460 399	2.4 0.8 1.4 1.0 2 1.8 2.0	10.5 6.0 7.6 7.5 9 8 12	
Methane Methanethiol Methanol 2-Methoxyethyl acetate Methyl acetate Methyl acrylate Methylamine 2-Methyl-2-butanol 3-Methyl-1-butene Methylcyclohexane Methyl formate 2-Methylpropene	540 385 502 430 437 365 250 465 465	5.4 3.9 6.7 1.7 3.1 2.8 4.9 1.2 1.5 1.2 5.0	15.0 21.8 36.0 8.2 16 25 20.6 9.0 9.1 6.7 23 9.6	
4-Methyl-2-pentanone 2-Methylpropene α-Methylstyrene Methyl propionate Nicotine	460 465 574 469 244	1.4 1.8 1.9 2.5	9.6 7.5 9.6 6.1 13	
Nitrobenzene Nonane	482 205	1.8 (93 °C) 0.8	2.9	
Octane	220	1.0	6.5	

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TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

		Flammable limits, percent by volume of fuel (25 °C, 760 mm)		
Substance	Autoignition temperature, °C	Lower	Upper	
Pentanamine		2.2	22	
Pentane	260	1.5	7.8	
2-Pentanone	505	1.5	8.2	
Pentyl acetate	360	1.1	7.5	
Petroleum ether	550	1.1	5.9	
Propane	450	2.2	9.5	
1,3-Propanediol	371	2.6	12.5	
Propanol	440	2.1	13.5	
Propene	460	2.0	11.1	
Propanamine	318	2.0	10.4	
Propionaldehyde	207	2.9	17.0	
Propyl acetate	450	2.0	8	
Propylene oxide		2.8	37.0	
Propyl nitrate	175	2	100	
Pyridine	482	1.8	12.4	
Styrene	490	1.1	6.1	
Tetrahydrofuran	321	2	11.8	
Tetrahydrofurfuryl alcohol	282	1.5	9.7	
Tetrahydronaphthalene	385	0.8	5.0	
Toluene	480	1.2	7.1	
Trichlorothylene	420	12.5	90	
Triethylamine		1.2	8.0	
Triethylene glycol	371	0.9	9.2	
Trimethylamine	190	2.0	11.6	
Trioxane	414	3.6	29	
Vinyl acetate	427	2.6	13.4	
Vinyl butyrate		1.4	8.8	
Vinyl chloride	461	3.6	33.0	
Vinyl fluoride		2.6	21.7	
Xylene, m- and p-	530	1.1	7.0	
Xylene, o-	465	1.0	6.0	

SECTION 5

THERMODYNAMIC PROPERTIES

	AND GIBBS (FREE) ENERGIES OF FORMATION,	
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5.2 SECTION 5

ENTHALPIES AND GIBBS (FREE) ENERGIES OF FORMATION, ENTROPIES, AND HEAT CAPACITIES

The tables in this section contain values of the enthalpy (ΔHf) and Gibbs (ΔGf) , free) energy of formation, entropy (S), and heat capacity (C_p) at 298.15 K (25 °C). The tables cover common organic compounds. No values are given in these tables for metal alloys or other solid solutions, for fused salts, or for substances of undefined chemical composition.

For a more complete listing of compounds see the tables in *Selected Values of Chemical Thermodynamical Properties*, by D. D. Wagman *et al.*, *National Bureau of Standards Technical Notes* 270-3, 270-4, 270-5, 270-6, 270-7, and 270-8, Washington; *JANAF Thermochemical Tables*, by D. R. Stull and H. Prophet, *National Bureau of Standards Publication 37*, Washington; supplements to JANAF appearing in *J. Phys. Chem. Ref. Data*; D. R. Stull, E. F. Westrum, Jr., and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds*, Wiley-Interscience, New York, 1969; and I. Barin and O. Knacke, *Thermochemical Properties of Inorganic Substances*, Springer-Verlag, Berlin, 1973.

The values of the thermodynamic properties of the pure substances given in these tables are, for the substances in their standard states, defined as follows:

Pure solid (c) or liquid (liq). The substance is in the condensed phase under a pressure of 1 atm.

Gas (g). The standard state is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure.

The values of ΔHf° and ΔGf° given in the tables represent the change in the appropriate thermodynamic quantity when one gram formula weight of the substance in its standard state is formed, isothermally at the indicated temperature, from the elements, each in its appropriate standard reference state. The standard reference state at 25 °C for each element has been chosen to be the standard state that is thermodynamically stable at 25 °C and 1 atm pressure. The standard reference states are indicated in the tables by the fact that the values of ΔHf° and ΔGf° are exactly zero.

The values of S° represent the virtual or "thermal" entropy of the substance in the standard state at 298.15 K, omitting contributions from nuclear spins. Isotope mixing effects are also excluded except in the case of the ${}^{1}\text{H}{}^{-2}\text{H}$ system.

The physical state of each substance is indicated in the column headed "State" as crystalline solid (c), liquid (liq), gaseous (g), or amorphous (amorp). Solutions in water are listed as aqueous (aq). Solutions in water are designated as aqueous, and the concentration of the solution is expressed in terms of the number of moles of solvent associated with 1 mol of the solute. If no concentration is indicated, the solution is assumed to be dilute. The standard state for a solute in aqueous solution is taken as the hypothetical ideal solution of unit molality (indicated as std state, m=1). In this state the partial molal enthalpy and the heat capacity of the solute are the same as in the infinitely dilute real solution (aq. m).

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	C_p° , cal $\cdot \deg^{-1} \cdot$ mol ⁻¹
Acenaphthene	С	16.8			
Acenaphthylene	С	44.7			
Acetaldeyde	liq	-45.96	-30.64	38.3	65.6
•	g	-39.76	-31.86	63.15	13.06
Acetaldoxime	c	-18.6			
	liq	-19.5			
Acetamide	c	-76.0			
Acetamidoguanidine nitrate	С	-118.1			
1-Acetamido-2- nitroguanidine	С	-46.3			
5-Acetamidotetrazole	с	-1.2			
Acetanilide	С	-50.3			
Acetic acid	liq	-115.71	-93.2	38.2	29.7
	g	-103.93	-90.03	67.52	15.90
Ionized; std state, $m = 1$	aq	-116.16	-88.29	20.7	-1.5
Nonionized; std state, $m = 1$	aq	-116.70	-94.78	42.7	
Acetic anhydride	liq	-149.14	-116.82	64.2	
	g	-137.60	-113.93	93.20	23.78
Acetone	liq	-59.18	-37.22	47.9	30.22
	g	-51.78	-36.58	70.49	17.90
Acetone glyceraldehyde	liq	-180			
Acetonitrile	liq	12.8	23.7	35.76	21.86
	g	21.00	25.24	58.19	12.48
Acetophenone	liq	-34.07	-4.06	59.62	
	g	-20.76	0.44	89.12	
Acetyl radical	g	-4.0			
N-Acetylbenzidine	С	-38.0			
Acetyl bromide	liq	-53.5	40.70	40.0	
Acetyl chloride	liq	-65.44	-49.73	48.0	28
A 1	g	-58.30	-46.29	70.47	16.21
Acetylene	g	54.19	50.00	48.00	10.50
Std state, $m = 1$	aq	50.54	51.88	29.5	
Acetylenedicarbonitrile	liq	119.6	122 10	60.21	20.52
Acetylene dicarboxylic acid	g c	127.50 -138.1	122.10	69.31	20.53
Acetyl fluoride	liq	-112.4			
N-Acetylhydrazobenzene	riq c	-112.4 -2.0			
o-Acetylhydroxybenzoic acid	c	-2.0 -194.93			
N-Acetylimidazole	с	-28.6			
Acetyl iodide	liq	-39.3			
4-Acetylresorcinol	С	-137.1			

5.4 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

	1	I	I	I	I
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	C_p° , cal · deg ⁻¹ · mol ⁻¹
<i>N</i> -Acetyltetrazole	С	19.49			
Acridine	c	44.8			
Acrolein	liq	-29.97	-16.17		
	g	-20.50	-15.45		
Acrylic acid	liq	-91.8			
	g	-80.36	-68.37	75.29	18.59
Acrylonitrile	liq	36.1			
	g	44.20	46.68	65.47	15.24
Adenine	С	23.21	71.58	36.1	
Adipic acid	С	-237.60			
	liq	-235.51	-177.17		
Aetioporphyrin I	С	-6.0			
Aetioporphyrin II	С	0.4			
α -Alanine					
D	С	-134.03	-88.23	31.6	
L	c	-133.96	-88.49	30.88	
DL	С	-134.55	-88.92	31.6	
Alanine anhydride	c	-128.0			
α -Alanylglycine					
DL	С	-185.64	-117.00	51.0	
L	С	-197.52	-127.30	46.62	
DL-Alanylphenylalanine	С	-170.2			
Alanylphenylalanyl	С	-89.3			
anhydride		171.50	-106.65	46.6	
Allantoin (5 ymaidahydantain)	С	-171.50	-100.03	40.0	
(5-ureidohydantoin) Allomucic acid		-142			
Alloxan monohydrate	С	-142 -239.08	-182.08	44.6	
Alloxantin dihydrate	c c	-510.3	-162.06	44.0	
Allyl radical		38			
1-Allyl-5-allylamino-	g c	83.7			
tetrazole		03.7			
1-Allyl-5-aminotetrazole	c	63.4			
2-Allyl-5-aminotetrazole	c	67.6			
Allyl chloride		-0.15	10.42	73.29	18.01
Allylcyclopentane	g liq	-15.74	10.42	13.29	16.01
Allyl ethyl sulfoxide	liq	-41.83			
Allyl trichloroacetate	liq	-94.5			
Amalic acid	c	-367.0			
Amarine	c	63			
<i>p</i> -Aminoacetophenone	c	70.2			
3-Aminoacridine	c	39.8			
5-Aminoacridine	c	38.1			
2-Aminobenzoic acid	c	-95.8			
3-Aminobenzoic acid	c	-98.2			
5 / Illimiocenzoic acid		70.2			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
4-Aminobenzoic acid	С	-98.8			
2-Aminobiphenyl	c	26.8			
4-Aminobiphenyl	c	19.4			
1-Aminobutane (butylamine)	liq	-30.52			
	g	-22.00	11.76	86.76	28.33
2-Aminobutane (<i>sec</i> - butylamine)	g	-24.90	9.71	83.90	27.99
4-Aminobutanoic acid	С	-138.1			
2-Aminoethanesulfonic acid	С	-187.7	-134.3	36.8	33.6
Ionized; std state, $m = 1$	aq	-171.92	-121.76	47.8	
Nonionized; std state, $m = 1$	aq	-181.92	-134.12	55.7	
2-Aminohexanoic acid (norleucine)	С	-152.7			
4-Aminohexanoic acid	c	-154.5			
5-Aminohexanoic acid	c	-153.7			
6-Aminohexanoic acid	c	-152.7			
3-Amino-2-methylpropane (2-butylamine)	liq	-31.68			
5-Aminopentanoic acid	c	-144.5			
5-Aminotetrazole	c	49.7			
5-Aminotetrazole nitrate	c	-6.6			
3-Amino-1,2,4-triazole	c	18.4			
Amygdalin	c	-455			
1,2-Anyhydroglucose- 3,5,6-triacetate	С	-411.7			
Aniline	liq	7.55	35.63	45.72	45.90
	g	20.76	39.84	76.28	25.91
Anisine	c	-51			
Anisoyl glycine	С	-180.9			
Anthracene	С	29.0	68.30	49.58	49.7
9,10-Anthracenedione	c	-49.6			
β -D-Arabinose	c	-252.84			
β -L-Arabinose	С	-252.84			
D-Arabonic acid-γ-lactone	С	-238.2			
L-Arginine	С	-148.66	57.40	50.0	
D-Arginine	c	-149.05	-57.43	59.9	
L-Ascorbic acid	С	-278.34			
(vitamin C)		-188.50	-126.73	41.7	
L-Asparagine L-Aspartic acid	c c	-232.47	-126.73 -174.53	40.66	
Azobenzene		232.71	177.55	10.00	
cis	с	86.7			
trans	c	76.6			

5.6 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol $^{-1}$	S° , cal · deg ⁻¹ · mol ⁻¹	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Azodicarbamide	С	-69.90			
Azulene	g	66.90	84.10	80.75	30.69
Barbituric acid	c	-152.2			
Benzaldehyde	liq	-21.23	2.24		
Benzuidenyde	g	-9.57	5.85		
Benzamide	c	-48.42	0.00		
Benzanilide	С	-22.3			
1,2-Benzanthracene	c	41			
2,3-Benzanthracene	c	38.3	85.79	51.48	
1,2-Benzanthra-9,10- quinone	c	-55.4			
Benzene	liq	11.71	29.72	41.41	19.52
	g	19.82	30.99	64.34	
Benzenethiol (thiophenol)	liq	15.32	32.02	53.25	41.40
	g	26.66	35.28	80.51	25.07
Benzidine	c	16.9			
Benzil	c	-36.8			
Benzoic acid	c	-92.03	-58.62	40.05	34.97
Benzoic anhydride	c	-103.0			
Benzonitrile	g	52.30	62.33	76.73	26.07
Benzophenone	c	-8.0	33.5	58.6	
<i>p</i> -Benzoquinone	c	-44.33			
Benzotriazole	С	59.74			
DL-Benzoylalanine	c	-147.9			
Benzoyl bromide	liq	-25.58			
Benzoyl chloride	liq	-39.17			
Benzoyl iodide	liq	-12.31			
Benzoylphenylalanine	С	-129.6			
Benzoyl sarcosine	С	-135.7			
3,4-Benzphenanthrene	С	44.2			
Benzyl radical	g	45 -38.49	-6.57	51.8	
Benzyl alcohol	liq	5.6	-0.37	31.6	
Benzyl bromide (2-bromotoluene)	liq	3.0			
Benzyl chloride	liq	-7.8			
<i>N</i> -Benzyldiphenylamine	c	44.2			
Benzyl ethyl sulfide	liq	-1.17			
Benzyl iodide	liq	13.8			
Benzyl mercaptan	liq	10.4			
Benzyl methyl ketone	liq	-36.30			
Benzyl methyl sulfide	liq	6.27			
Bicyclo[4.1.0]heptane	g	0.33			
Bicyclo[3.1.0]hexane	g	9.09			
Bicyclo[4.2.0]octane	g	-6.39			
Bicyclo[5.1.0]octane	g	-3.85			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ},$ kcal·mol $^{-1}$	S° , $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot \operatorname{mol}^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Bicyclopropyl	g	30.9			
Biphenyl	С	24.02	60.75	49.2	38.80
	liq	28.5	62.07	59.8	
Biphenylene	liq	84.4			
<i>N</i> , <i>N</i> ′-Bisuccinimide	c	-169.5			
Brassidic acid	c	-214			
Bromal	liq	-31.13			
Bromal hydrate	c	-112			
Bromobenzene	liq	14.5	30.12	52.0	37.17
4-Bromobenzoic acid	c	-90.4			
1-Bromobutane	g	-25.65	-3.08	88.39	26.13
2-Bromobutane	liq	-37.2	-4.60		
	g	-28.70	-6.16	88.50	26.48
Bromochlorodi-	g	-112.7	-107.18	76.14	
fluoromethane					
Bromochloro-	g	-70.5	-66.58	72.88	
fluoromethane	0				
Bromochloromethane	g	-12.0	-9.39	68.67	
Bromodichloro-	g	-64.4	-58.98	78.87	
fluoromethane	8				
Bromodichloromethane	g	-14.0	-10.16	75.56	
Bromodifluoromethane	g	-110.8	-106.90	70.51	
Bromoethane	liq	-21.99	-6.64	47.5	24.1
Diomoculation .	g	-15.30	-6.29	68.71	15.45
Bromoethene	g	18.73	19.30	65.83	13.26
(vinyl bromide)	5	10.75	17.50	03.03	13.20
Bromofluoromethane	g	-60.4	-57.71	65.97	
1-Bromoheptane	liq	-52.21	37.71	03.77	
1-Bromohexane	liq	-46.42			
Bromoiodomethane	g	12.0	9.36	73.49	
Bromomethane	g	-9.02	-6.75	58.76	10.15
2-Bromo-2-methylpropane	liq	-39.3	0.75	30.70	10.13
2 Bromo 2 metny propane	g	-32.00	-6.73	79.34	27.85
1-Bromooctane	liq	-58.57	0.73	17.54	27.03
1-Bromopentane	liq	-40.68			
1-Bromopentane	*	-30.87	-1.37	97.70	31.60
1 Promonronono	g	-21.00	-5.37	79.08	20.66
1-Bromopropane 2-Bromopropane	g	-23.20	-6.51	75.53	21.37
N-Bromosuccinimide	g c	-80.35	-0.51	13.33	21.37
			_2.06	70.55	
Bromotrichloromethane	g	-8.9 -155.1	-2.96 -148.8	79.55	16.57
Bromotrifluoromethane Brucine	g	-155.1 -188.6	-148.8	71.16	16.57
	С	-188.6	47.42	70.02	10.15
1,2-Butadiene	g	38.77	47.43	70.03	19.15
1,3-Butadiene	g	26.33	36.01	66.62	19.01
Butadiyne (biacetylene)	g	113.00	106.11	59.76	17.60

5.8 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		I		1	I
		A 7700	A G (0)	S°,	C_p° ,
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	$cal \cdot deg^{-1} \cdot mol^{-1}$	cal·deg ⁻¹ ·mol ⁻¹
Butane	liq	-35.29	-3.60	55.2	
	g	-30.15	-4.10	74.12	23.29
1,2-Butanediamine	liq	-28.74			
2,3-Butanedione (diacetyl)	liq	-87.44			
1,4-Butanedithiol	liq	-25.11			
1-Butanethiol	liq	-29.79	0.97	65.96	
(butyl mercaptan)					
	g	-21.05	2.64	89.68	28.24
2-Butanethiol	liq	-31.13	-0.04	64.87	
	g	-23.00	1.29	87.65	28.51
1-Butanol	liq	-78.18	-38.84	54.1	42.31
	g	-65.65	-36.04	86.7	26.29
2-Butanol	liq	-81.88	-42.31	53.8	47.5
	g	-69.94	-40.06	85.6	27.08
2-Butanone	liq	-65.29	-36.18	57.08	37.98
(methyl ethyl ketone)					
	g	-56.26	-34.91	80.81	24.59
1-Butene	g	-0.03	17.04	73.04	20.47
2-Butene					
cis	g	-1.67	15.74	71.90	18.86
trans	g	-2.67	15.05	70.86	20.99
1-Buten-3-yne	g	72.80	73.13	66.77	17.49
tert-Butoxy radical	g	-24.7			
tert-Butyl radical	g	6.7			
N-Butylacetamide	liq	-91.02			
Butyl acetate	liq	-126.52			
tert-Butylamine	liq	-35.97			
	g	-28.65	6.90	80.76	28.67
Butylbenzene	liq	−18.67 ¹⁸ °C	27.50		
	g	-3.30	34.58	105.04	41.85
sec-Butylbenzene	liq	-15.87			
tert-Butylbenzene	liq	-16.90			
sec-Butyl butyrate	liq	-141.6			
Butyl chloroacetate	liq	-128.7			
Butyl 2-chlorobutyrate	liq	-156.6			
Butyl 3-chlorobutyrate	liq	-146.0			
Butyl 4-chlorobutyrate	liq	-147.7			
Butyl 2-chloropropionate	liq	-136.7			
Butyl 3-chloropropionate	liq	-133.4			
Butyl crotonate	liq	-111.8 -50.05	12.40	100.50	40.50
Butylevelenentene	g	-50.95	13.49	109.58	49.50
Butylcyclopentane	g lia	-40.22 -121.5	14.67	109.04	42.42
Butyl dichloroacetate Butyl ether	liq liq	-131.5 -156.1			
Daily I Chief	liq	-136.1 -87.2	114.96	48.82	
tert- Butyl hydroperoxide	g liq	-87.2 -70.2	114.90	40.04	
	_				

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Butyllithium	liq	-31.6			
Butyl trichloroacetate	liq	-130.6			
1-Butyne (ethyl acetylene)	g	39.48	48.30	69.51	19.46
2-Butyne	g	34.97	44.32	67.71	18.63
(dimethylacetylene)	_				
Butyraldehyde	g	-49.00	-27.43	82.44	24.52
Butyramide	c	-87.5			
Butyric acid	liq	-127.59	-90.27	54.1	42.1
Butyronitrile	g	8.14	25.97	77.98	23.19
Caffeine	С	-76.2			
(methyl theobromine)					
Capric acid (decanoic acid)	с	-170.59			
Caproic acid (hexanoic acid)	liq	-139.71			
ε-Caprolactam	С	-78.54	-22.72	40.3	
Caprylic acid	liq	-151.93			
(octanoic acid)	_				
Carbazole	c	30.3			
Carboxyl radical	g	-54			
CCH radical	g	114	105	49.6	8.87
Cellobiose	С	-532.5			
Chloroacetamide	c	-80.9			
Chloroacetic acid	c, 1	-122.3			
Ionized	aq	-119.81			
Nonionized; std state, $m = 1$	aq	-118.92			
Chloroacetyl chloride	liq	-68.0			
2-Chlorobenzaldehyde	liq	-28.4			
3-Chlorobenzaldehyde	liq	-30.2			
4-Chlorobenzaldehyde	С	-35.1			
Chlorobenzene	liq	2.58	21.32	50.0	35.9
2-Chlorobenzoic acid	С	-95.3			
3-Chlorobenzoic acid	С	-101.2			
4-Chlorobenzoic acid	С	-102.19			
Chlorobenzoquinone	С	-52.7			
1-Chlorobutane	g	-35.20	-9.27	85.58	25.71
2-Chlorobutane	g	-38.60	-12.78	85.94	25.93
2-Chlorobutyric acid	liq	-137.6			
3-Chlorobutyric acid	liq	-133.0			
4-Chlorobutyric acid	liq	-135.4			
Chlorocyclohexane	liq	-49.54	72.00	72.20	
2-Chloro-1,1-	g	-79.2	-72.90	72.28	
difluoroethylene Chlorodifluoromethane	g	-115.6	-108.1	67.12	13.35

5.10 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		$\Delta H f^{\circ}$,	$\Delta G f^{\circ}$,	S° , cal · deg ⁻¹ ·	C_p° , cal $\cdot \deg^{-1} \cdot$
Substance	State	kcal·mol ⁻¹	kcal·mol ⁻¹	mol ⁻¹	mol ⁻¹
Chloroethane (ethyl chloride)	g	-26.83	-14.46	65.91	14.97
Chloroethylene (vinyl chloride)	g	8.5	12.4	63.07	12.84
Chloroethyne	g	51	47	57.81	12.98
Chlorofluoromethane	g	-63.2	-57.11	63.16	11.24
Chloroform	liq	-31.6	-17.17	48.5	
	g	-24.60	-16.76	70.63	15.63
Chloroiodomethane	g	3.0	3.69	70.78	
Chloromethane (methyl chloride)	g	-19.59	-13.97	55.97	9.74
Chloromethyloxirane	liq	-35.48			
1-Chloro-2-methylpropane	g	-38.10	-11.87	84.56	25.93
2-Chloro-2-methylpropane	g	-43.80	-15.32	77.00	27.30
1-Chloronaphthalene	liq	13.0			
2-Chloronaphthalene	c	13.2			
1-Chloropentane	g	-41.80	-8.94	94.89	31.18
3-Chorophenol	С	-49.4			
4-Chlorophenol	С	-47.3			
1-Chloropropan-2,3-diol	liq	-125.58			
2-Chloropropan-1,3-diol	liq	-123.71			
1-Chloropropane	g	-31.10	-12.11	76.27	20.23
2-Chloropropane	g	-35.00	-14.94	72.70	20.87
3-Chloro-1-propene (allyl chloride)	g	-0.15	10.42	73.29	18.01
2-Chloropropionic acid	liq	-125.0			
3-Chloropropionic acid	c	-131.4			
N-Chlorosuccinimide	С	-85.58			
Chlorotrifluoromethane	g	-169.20	-159.38	68.16	15.98
Chlorotrinitromethane	liq	-6.54			
Chrysene	С	34.7			
Cinchonamine	С	-10.4			
Cinchonidine	С	7.1			
Cinchonine	С	7.4			
Cinnamic acid	_	72.0			
cis trans	c c	-72.0 -80.53			
Cinnamic anhydride	c	-83.1			
Citraconic acid	c	-197.04			
Citric acid	c	-369.0	-295.5	39.73	
Citric acid monohydrate	c	-439.4	-352.0	67.74	1.276
Codeine monohydrate	c	-151.2	222.0		1.2,0
Coniine	liq	-57.6			
Creatine	c	-128.16	-63.32	45.3	
Creatine hydrate	c	-199.1			
Creatinine	c	-56.77	-6.97	40.10	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ},$ kcal·mol $^{-1}$	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
o-Cresol	g	-30.74	-8.86	85.47	31.15
(2-methylphenol) m-Cresol (3-methylphenol)	g	-31.63	-9.69	85.27	29.27
<i>p</i> -Cresol (4-methylphenol)	g	-29.97	-7.38	83.09	29.75
m-Cresol acetate Crotonic acid	liq	-89.41			
cis	liq	-83			
trans	С	-102.9	46.22	71.21	10.62
trans-Crotononitrile	g	35.77 14.05	46.22	71.31	19.62
Cyanamide 1-Cyanoguanidine	c c	5.4	42.9	30.90	28.40
3-Cyanopyridine	c	46.23	42.9	30.90	20.40
5-Cyanotetrazole	c	96.1			
4-Cyanothiazole	c	52.63			
Cyclobutane	g	6.37	26.30	63.43	17.26
Cyclobutene	g	31.00	41.76	62.98	16.03
Cyclododecane	c	-73.29	111,0	02.70	10.02
Cycloheptane	liq	-37.47	12.92	57.97	29.42
Cycloheptanone	liq	-71.5			
1,3,5-Cycloheptatriene	liq	34.22	58.09	51.30	38.90
1,3-Cyclohexadien-5-yl radical	g	49.4			
Cyclohexane	liq	-37.34 -29.43	6.37	48.84	37.4 25.40
Cyclohexane- 1,2- dicarboxylic acid	g		7.59	71.28	23.40
cis	С	-229.7			
trans	С	-232.0			
Cyclohexanethiol	g	-22.80	24.05		
Cyclohexanol	liq	-83.22	-31.87	47.7	26.21
Cyclohexanone	g 1:-	-55.00	-21.69	77.00	26.21
Cyclohexene	liq	-9.28	24.28	51.67	34.9
Cycloboxon 2 vl modical	g	-1.28 29	25.54	74.27	25.10
Cyclohexen-3-yl radical 1-Cyclohexenylmethanol	g liq	-91.4			
Cyclohexyl radical		13			
Cyclooctane	g liq	-40.58	18.60	62.62	
Cyclooctanone	liq	-77.9	10.00	02.02	
1,3,5,7-Cyclooctatetraene	liq	60.93	85.70	52.65	
Cyclopentadiene	g	32.00	42.86	64.00	
Cyclopentane	liq	-25.28	8.70	48.82	30.80
- 7 · · F	g	-18.46	9.23	70.00	19.84
Cyclopentane-1,2-diol					
* *	c	-115.9			
cis		110.7			

5.12 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		I			
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	C_p° , cal $\cdot \deg^{-1} \cdot \gcd^{-1}$
Cyclopentanethiol	g	-11.45	13.63	86.38	25.79
Cyclopentanol	liq	-71.74	-30.55	49.2	23.77
Cyclopentanone	liq	-56.24	30.33	17.2	
Cyclopentatione		-46.03			
Cyclopentene	g liq	1.02	25.93	48.10	29.24
Сусторениене	1 1	7.87	26.48	69.23	17.95
1 Cyclomontonyilmothomol	g	8.2	20.40	09.23	17.93
1-Cyclopentenylmethanol	liq	-15.41			
Cyclopentyl-1-thiaethane	g		24.05	56.75	12.27
Cyclopropane	g	12.74	24.95		13.37
Cyclopropene	g	66.0	68.42	58.38	
Cyclopropyl radical	g	55			
L-Cysteine	С	-124.5			
L-Cystine	С	-245.7			
Decahydronaphthalene (decalin)					
cis	liq	-52.45	16.47	63.34	55.45
trans	liq	-55.14	13.79	63.32	54.61
Decanal	g	-79.09	-15.90	138.28	57.29
Decane	liq	-71.95	-4.19	101.70	75.16
1,10-Decanediol	c 1	-165.74			
1-Decanethiol	liq	-66.07			
	g	-50.54	14.68	145.82	61.08
1-Decanoic acid	c	-170.59		- 1010-	0 2 1 0 0
1-Decanol	liq	-114.6	-31.6	10.2.9	
1 Decumen	g	-96.0	-24.9	142.8	59.1
1-Decene	liq	-41.73	25.10	101.58	57.1
1-Decyne	g	9.85	60.28	125.36	52.51
Deoxybenzoin	c	-16.96	00.20	123.30	32.31
Desoxyamalic acid	c	-285.7			
Diacetamide	c	-117			
Diacetyl peroxide	liq	-127.9			
o-Diallyl phthalate	liq	-131.6			
Dialuric acid	c	-314.4			
2,6-Diaminopyridine	c	-1.56			
Diamylose	c	-850			
Diazomethane		46.0	52.06	58.02	12.55
Dibenzoylethane	g c	-61.1	32.00	36.02	14.33
•	c	-01.1 -27.4			
Dibenzoylethylene Dibenzoylmethane		-53.6			
•	С	-53.6 -100			
Dibenzoyl peroxide	С		62.15	61.4	61.0
Dibenzyl	С	10.53	62.15	64.4	61.0
Dibenzyl ketone	С	-20.1			
Dibenzyl sulfide	С	23.74			
Dibenzyl sulfone	С	-42.1			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
1,2-Dibromobutane	g	-23.70	-3.14	97.70	30.38
Dibromochlorofluoro-	g	-55.4	-53.40	81.99	20.20
methane					
Dibromochloromethane	g	-5.0	-4.50	78.31	
1,2-Dibromocycloheptane	liq	-37.67			
1,2-Dibromocyclohexane	liq	-38.8			
1,2-Dibromocyclooctane	liq	-41.41			
Dibromodichloromethane	g	-7.0	-4.67	83.23	
Dibromodifluoromethane	g	-102.7	-100.16	77.66	22.54
1,2-Dibromoethane	liq	-19.4	-5.0	53.37	32.51
Dibromofluoromethane	g	-53.4	-52.84	75.70	12.04
Dibromomethane	g	-3.53	-3.87	70.10	13.04
1,2-Dibromopropane	g 1: -	-17.40	-4.22	89.90	24.57
Dibutylborinic acid Dibutyl ether	liq	-146.3 -79.80	-21.16	119.60	48.76
Dibutyl ether Dibutylmercury	g liq	-79.80 -23.4	-21.16	119.00	46.70
Di- <i>tert</i> -butyl peroxide	liq	-23.4 -91.0			
Dibutyl <i>o</i> -phthalate	c	-201			
Dibutyl sulfate	liq	-216.1			
Dibutyl sulfite	liq	-165.6			
Dibutyl sulfone	c	-145.76			
Dichloroacetic acid	liq	-119.0			
Ionized	aq	-122.4			
Nonionized	aq	-120.4			
Dichloroacetylene	g	50	47	65	15.67
1,2-Dichlorobenzene	g	7.16	19.76	81.61	27.12
1,3-Dichlorobenzene	g	6.32	18.78	82.09	27.20
1,4-Dichlorobenzene	g	5.50	18.44	80.47	27.22
Dichlorodifluoromethane	g	-117.90	-108.51	71.91	17.31
1,1-Dichloroethane	liq	-38.3	-18.1	50.61	30.18
	g	-31.10	-17.52	72.91	18.25
1,2-Dichloroethane	liq	-39.49	-19.03	49.84	30.9
	g	-31.00	-17.65	73.66	18.80
1,1-Dichloroethylene	liq	-5.8	5.85	48.17	26.60
	g	0.30	5.78	68.85	16.02
cis-1,2-Dichloroethylene	liq	-6.6	5.27	47.42	27
4.6.51.11	g	0.45	5.82	69.20	15.55
trans-1,2-Dichloroethylene	_	1.00	6.35	69.29	15.93
Dichlorofluoromethane	g 1: -	-68.10	-60.77	70.04	14.58
Dichloromethane	liq	-29.7	-16.83	42.7	12.16
1.2 Diahlamamanana	g	-22.80	-16.46	64.61	12.16
1,2-Dichloropropane	g	-39.60 -38.60	-19.86 -19.74	84.80 87.76	23.47 23.81
1,3-Dichloropropane 2,2-Dichloropropane	g	-38.60 -42.00	-19.74 -20.21	77.92	25.30
Dicyanoacetylene	g liq	119.6	-20.21	11.94	25.30
	114	117.0			

5.14 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

				S°,	C_p° ,
Substance	State	ΔHf° , kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	$cal \cdot deg^{-1} \cdot mol^{-1}$	cal · deg ⁻¹ · mol ⁻¹
1,4-Dicyano-2-butyne	С	87.6			
Dicyclohexadiene	liq	6.3			
Dicyclopentadiene	c	27.9			
Dicyclopentyl	liq	-41.8			
2,2-Diethoxypropane	liq	-128.83			
Diethylamine	g	-17.30	17.23	84.18	27.66
Diethylbarbituric acid (veronal)	С	-178.7			
1,2-Diethylbenzene	g	-4.53	33.72	103.81	43.63
1,3-Diethylbenzene	g	-5.22	32.67	104.99	42.27
1,4-Diethylbenzene	g	-5.32	32.95	103.73	42.10
Diethylenediamine	С	-3.2	57.4	20.5	
Diethylene glycol	liq	-150.2			
	g	-136.5		105.4	32.3
Diethyl ether (ethyl ether)	liq	-65.30	-27.88	60.5	40.8
	g	-60.26	-29.24	81.90	26.89
Diethylmercury	liq	7.1			
Diethylmethyl phos- phonate	liq	-245.3			
Diethylnitramine	liq	-25.4			
Diethyl oxalate	liq	-192.51			
Diethyl peroxide	liq	-53.4			
Diethyl o-phthalate	liq	-186			
Diethyl selenide	liq	-23.0			
Diethyl sulfate	liq	-194.28			
Diethyl sulfite	liq	-143.50			
Diethyl sulfone	c	-123.13			
Diethyl sulfoxide	liq	-63.97			
Diethylzinc	liq	4.0	50.41	52.20	20.01
1,2-Difluorobenzene	liq	-79.04	-59.41	53.20	38.01
1,3-Difluorobenzene	g	-74.09	-61.43	76.57	25.40
1,4-Difluorobenzene	g	-73.43	-60.43	75.43	25.55
2,2'-Difluorobiphenyl	С	-70.73			
4,4-Difluorobiphenyl 2,2-Difluorochloroethylene	С	-70.91 -75.4	-69.1	72.39	17.23
1,1-Difluoroethane	g	-73.4 -119.70	-105.87	67.50	16.24
1,1-Difluoroethylene	g	-82.50	-76.84	63.38	14.14
Difluoromethane	g	-82.30 -108.24	-70.84 -101.66	58.94	10.25
9,10-Dihydroanthracene	g c	15.87	101.00	30.74	10.23
1,2-Dihydronaphthalene	liq	18.0			
1,4-Dihydronaphthalene	liq	21.0			
4 <i>H</i> -Dihydropyran	liq	-37.5			
5,12-Dihydrotetracene	c	25.44			
2,3-Dihydrothiophene	liq	12.73			
, ,	1				

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
2,5-Dihydrothiophene	liq	11.31			
1,2-Dihydroxybenzene	c	-86.3	-50.20	35.9	31.6
1,3-Dihydroxybenzene	С	-87.95	-50.00	35.3	31.3
1,2-Diiodobenzene	С	41.2			
1,3-Diiodobenzene	С	44.7			
1,4-Diiodobenzene	С	38.4			
1,2-Diiodoethane	g	15.90	18.76	83.30	19.67
Diiodomethane	g	28.30	24.24	73.95	13.80
Diisopropyl ether	liq	-83.94	-21.1	70.4	
1 1	g	-76.20	-29.13	93.27	37.83
Diisopropyl ketone	g	-74.40			
Diisopropylmercury	liq	-3.1			
1,2-Dimethoxybenzene	liq	-69.4			
Dimethoxyborane	liq	-144.5			
1,2-Dimethoxyethane	liq	-90.02			
2,2-Dimethoxypropane	liq	-108.92			
$cis-\alpha,\beta$ -Dimethylacrylic acid	c	-117.3			
Dimethyl adipate	liq	-211.9			
Dimethylamine	g	-4.50	16.25	65.24	16.50
Std state, $m = 1$	aq	-16.88	13.85	31.8	
(CH ₃) ₂ NH ₂ ⁺ ;	aq	-28.74	-0.80	41.2	
std state, $m = 1$	_				
Dimethylaminotrimethyl- silane	liq	-66.8			
N,N-Dimethylaniline	liq	8.2			
2,2-Dimethylbutane	g	-44.35	-2.20	85.62	33.91
2,3-Dimethylbutane	g	-42.49	-0.98	87.42	33.59
2,3-Dimethyl-1-butene	g	-13.32	18.89	87.39	34.29
2,3-Dimethyl-2-butene	g	-14.15	18.18	87.15	29.54
3,3-Dimethyl-1-butene	g	-10.31	23.46	82.16	30.23
2,3-Dimethyl-2-butenoic acid	c	-108.9			
Dimethylcadmium	g	9.528		72.40	31.5
Dimethylchlorosilane	liq	-79.8			
1,1-Dimethylcyclohexane	liq	-52.31	6.34	63.87	
	g	-43.26	8.42	87.24	36.90
1,2-Dimethylcyclohexane					
cis	g	-41.15	9.85	89.51	37.40
trans	g	-43.02	8.24	88.65	38.00
1,3-Dimethylcyclohexane					
cis	g	-44.16	7.13	88.54	37.60
trans	g	-42.20	8.68	89.92	37.60
1,4-Dimethylcyclohexane	5				
cis	g	-42.22	9.07	88.54	37.60
trans	g	-44.12	7.58	87.19	37.70
<i>u w to</i>	5	77.12	7.50	07.17	37.70

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						
1,2-Dimethylcyclopentane	Substance	State			$cal \cdot deg^{-1} \cdot$	cal · deg ⁻¹ ·
cis trans g g -30.96 -32.67 10.93 9.17 87.67 87.67 32.14 32.14 1.3-Dimethylcyclopentane cis trans g -32.47 g 9.37 9.91 87.67 87.67 32.14 32.14 Dimethyldichlorosilane cis-2,4-Dimethyl-1,3-dioxane 4,5-Dimethyl-1,3-dioxane smine Dimethyl ether liq g -110.2 -110.53 80.16 24.17 4,5-Dimethyl-1,3-dioxane smine Dimethyl ether g -43.99 -2.8 -26.99 63.83 63.83 15.73 15.73 N,N-Dimethylformamide Dimethyl flumarate Dimethyl flumarate Dimethyl glutarate Dimethyl glutarate Dimethyl flumarate Dimethyl glutarate Dimethylhexane 2,2-Dimethylhexane 2,3-Dimethylhexane g liq g -55.72 25.6 28.5 37.45 2,3-Dimethylhexane 2,4-Dimethylhexane g liq g -62.63 g 0.71 3.24 79.33 3.24 106.11 3.06 2.17 3.25 81.91 3.3-Dimethylhexane 106.11 104.93 3.3-Dimethylhexane 106.11 104.70 3.4-Dimethylhexane 106.11 107.15 2.2-Dimethylhexane 104 g 107.15 2.2-Dimethylhydrazine 104 107.15 2.2-Dimethylhydrazine 104 107.15 2.2-Dimethylhydrazine 104 107.15 104.70 3.4-Dimethylhydrazine 104 107.15 3.9.21 4.14 47.32 47.60 39.21 47.60 40.88 47.60 40.88 47.60 40.88 47.60		g	-33.05	9.33	85.87	31.86
1,3-Dimethylcyclopentane cis c		g	-30.96	10.93	87.51	32.06
1,3-Dimethylcyclopentane cis g -32.47 9.37 87.67 32.14 trans g -31.93 9.91 87.67 32.14 Dimethyldichlorosilane cis-2,4-Dimethyl-1,3-dioxane dioxane 110.2 80.16 24.17 4,5-Dimethyl-1,3-dioxane 5,5-Dimethyl-1,3-dioxane amine 1iq -110.53 4.4'-Dimethyldiphenylamine 1iq -110.53 4,4'-Dimethyldiphenylamine g -43.99 -26.99 63.83 15.73 N/N-Dimethylfulvene liq -57.2 28.5 37.45 Dimethyl fulware binethyl glyoxime c -22.8 28.5 37.45 Dimethylplexane binethyllexane liq -62.63 0.71 79.33 25.5 37.45 2,3-Dimethylhexane liq -60.40 2.17 81.91 23.3-Dimethylhexane g -51.13 4.23 106.11 24.23 106.11 24.24-Dimethylhexane g -52.44 2.80 106.51 25.5-Dimethylhexane g -53.21 2.50 104.93 3.3-Dimethylhexane g -53.21 2.50 104.93 3.4-Dimethylhexane g -52.61 3.17 </td <td>trans</td> <td></td> <td>-32.67</td> <td>9.17</td> <td>87.67</td> <td>32.14</td>	trans		-32.67	9.17	87.67	32.14
cis trams g g -32.47 31.93 9.37 9.91 87.67 87.67 32.14 32.14 Dimethyldichlorosilane cis-2,4-Dimethyl-1,3-dioxane 4,5-Dimethyl-1,3-dioxane 4,5-Dimethyl-1,3-dioxane 1,5-Dimethyl-1,3-dioxane 4,4'-Dimethyldiphenyl- amine liq liq 110.53 -110.2 -110.53 80.16 24.17 Dimethyl ether N/N-Dimethylformamide Dimethyl fulvare Dimethyl fulvarate Dimethyl glutarate Dimethyl glutarate Dimethyl glutarate Dimethylgyoxime 2,2-Dimethylhexane g -43.99 -22.8 -26.99 -28.5 63.83 37.45 15.73 37.45 2,3-Dimethylhexane 2,3-Dimethylhexane 2,4-Dimethylhexane 3,3-Dimethylhexane liq liq liq -61.47 -60.40 0.71 2.17 2.56 103.06 79.33 2.56 103.06 82.62 2.52-Dimethylhexane 82.62 2.52-Dimethylhexane 82.62 2.52-Dimethylhexane 82.62 2.52-Dimethylhexane 82.62 2.52-Dimethylhexane 106.11 2.42-Dimethylhexane 106.11 2.42-Dimethylhexane 106.11 2.43-Dimethylhexane 106.11 2.50 106.51 2.50 106.51 2.50 104.93 2.50 81.12 2.50 82.92 2.50 104.93 3.3-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 104.70 2.52-Dimethylhexane 107.15 107.15 2,2-Dimethylhexane 104.70 2.52-Dimeth	1,3-Dimethylcyclopentane					
Dimethyldichlorosilane cis-2,4-Dimethyldichlorosilane cis-2,4-Dimethyl-1,3-dioxane liq -110.79		g	-32.47	9.37	87.67	32.14
Dimethyldichlorosilane cis-2,4-Dimethyl-1,3- dioxane 4,5-Dimethyl-1,3-dioxane liq -110.53 4,4'-Dimethyl-1,3-dioxane liq -110.53 4,4'-Dimethyldiphenyl- amine Dimethyl tether g -43.99 -26.99 63.83 15.73 7.45 Dimethylfumarate liq -57.2 28.5 37.45 Dimethylfumarate liq -205.9 Dimethylguvane c -42.51 2.50 Dimethylguvane liq -62.63 0.71 79.33 g -53.71 2.56 103.06 2.3-Dimethylhexane liq -60.40 2.17 81.91 2.3-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2.5-Dimethylhexane liq -62.26 0.60 80.96 2.5-Dimethylhexane liq -61.58 1.23 81.12 3.3-Dimethylhexane liq -60.23 2.03 82.97 3.4-Dimethylhydantoin g -50.91 4.14 107.15 2.2-Dimethylhydrazine liq -34.64 5.5-Dimethylhydrazine liq -34.64 5.5-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1.2-Dimethylhydrazine liq -168.2 Dimethylmaleate liq -168.2 Dimethylmaleate liq -168.2 Dimethylmaleate liq -169.2 Dimethylmaleate liq -169.2 Dimethylmaleate liq -169.2 Dimethylmaleate liq -161.9 Dimethylmaleate liq -161.8 Dime	trans		-31.93	9.91	87.67	32.14
cis-2,4-Dimethyl-1,3-dioxane liq -111.79 4,5-Dimethyl-1,3-dioxane liq -108.32 5,5-Dimethyl-1,3-dioxane liq -110.53 4,4'-Dimethyldiphenyl-amine liq -170.53 Dimethyl ether g -43.99 -26.99 63.83 15.73 N,N-Dimethylformamide liq -57.2 28.5 37.45 Dimethyl flumarate liq -174.3 Dimethyl glydrame 28.5 37.45 Dimethyl glyoxime c -42.51 22.50 103.06 28.5 37.45 2,3-Dimethylhexane liq -62.63 0.71 79.33 79.33 2.56 103.06 103.06 2.3-Dimethylhexane g -51.13 4.23 106.11 106.11 2.4-Dimethylhexane g -51.13 4.23 106.11 106.11 106.51 2.2-Dimethylhexane liq -61.47 0.89 82.62 2.2-Dimethylhexane g -52.44 2.80 106.51 3.3-Dimethylhexane liq -61.58 1.23 81.12	Dimethyldichlorosilane		-110.2		80.16	24.17
5,5-Dimethyl-1,3-dioxane d.4'-Dimethyldiphenylamine liq c110.53 c2.8 c2.9 c2.8 c2.9 c.	•		-111.79			
4,4'-Dimethyldiphenylamine C -2.8	4,5-Dimethyl-1,3-dioxane	liq	-108.32			
amine Dimethyl ether Dimethyl formamide Dimethylfulvene Dimethylfulvene Dimethylfulvene Dimethylfulvene Dimethylfulvene Dimethylfulvene Dimethyl glutarate Dimethylglyoxime C 2,2-Dimethylhexane Liq C 3,3-Dimethylhexane Liq C 4,4-Dimethylhexane Liq C 5,5-Dimethylhexane Liq C C C C C C C C C C C C C C C C C C C	5,5-Dimethyl-1,3-dioxane	liq	-110.53			
N,N-Dimethylformamide Dimethylfulvene liq		c	-2.8			
Dimethylfulvene liq 21.5 Dimethyl fumarate liq -174.3 Dimethyl glutarate liq -205.9 Dimethylglyoxime c -42.51 2,2-Dimethylhexane liq -62.63 0.71 79.33 2,3-Dimethylhexane g -53.71 2.56 103.06 2,3-Dimethylhexane g -51.13 4.23 106.11 2,4-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -61.58 1.23 81.12 g -52.61 3.17 104.70 3,4-Dimethylhexane liq -60.23 2.03 82.97 g -50.91 4.14 107.15 2,2-Dimethylhydrazine liq -34.64 47.32 39.21 1,1-Dimethylhydrazine	Dimethyl ether	g	-43.99	-26.99	63.83	15.73
Dimethyl fumarate	N,N-Dimethylformamide	liq	-57.2		28.5	37.45
Dimethyl glutarate liq -205.9 Dimethylglyoxime c -42.51 2,2-Dimethylhexane liq -62.63 0.71 79.33 2,3-Dimethylhexane liq -60.40 2.17 81.91 2,3-Dimethylhexane g -51.13 4.23 106.11 2,4-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -62.26 0.60 80.96 g -53.21 2.50 104.93 3,3-Dimethylhexane liq -61.58 1.23 81.12 g -52.61 3.17 104.70 3,4-Dimethylhexane liq -60.23 2.03 82.97 g -50.91 4.14 107.15 2,2-Dimethyl-3-hexene cis liq -34.64 5,5-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 11.8 49.4 47.	Dimethylfulvene	liq	21.5			
Dimethylglyoxime c -42.51 79.33 2,2-Dimethylhexane liq -62.63 0.71 79.33 2,3-Dimethylhexane liq -60.40 2.17 81.91 2,3-Dimethylhexane g -51.13 4.23 106.11 2,4-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -62.26 0.60 80.96 g -53.21 2.50 104.93 3,3-Dimethylhexane liq -61.58 1.23 81.12 g -52.61 3.17 104.70 3,4-Dimethylhexane liq -60.23 2.03 82.97 g -50.91 4.14 107.15 2,2-Dimethyl-3-hexene liq -30.22 -34.64 5,5-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 11.3.3 50.8 47.60 40.88	Dimethyl fumarate	liq	-174.3			
2,2-Dimethylhexane liq g -62.63 g 0.71 (13.06) 79.33 (13.06) 2,3-Dimethylhexane liq (14.06) -60.40 (13.06) 2.17 (13.06) 81.91 (13.06) 2,3-Dimethylhexane g (14.06) -51.13 (13.06) 4.23 (106.11) 106.11 (16.11) 2,4-Dimethylhexane liq (16.47 (16.47)) 0.89 (16.51) 82.62 (16.51) 82.62 (16.51) 2,5-Dimethylhexane liq (16.58) 1.23 (16.51) 80.96 (16.51) 80.96 (16.51) 3,3-Dimethylhexane liq (16.58) 1.23 (16.51) 81.12 (16.51) 81.12 (16.51) 3,4-Dimethylhexane liq (16.58) 1.23 (16.51) 81.12 (16.51) 81.12 (16.51) 2,2-Dimethyl-3-hexene g (16.58) 1.23 (16.51) 81.12 (16.51) 82.97 (16.58) 2,2-Dimethyl-3-hexene liq (16.58) 1.31 (16.11) 104.70 (16.51) 104.70 (16.51) 2,2-Dimethylhydrazine liq (16.58) 1.14 (16.51) 107.15 (16.51) 2,2-Dimethylhydrazine liq (16.58) 1.23 (16.51) 104.70 (16.51) 3,4-Dimethylmaleate liq (16.51) 1.18 (16.51) 104.70 (16.51)	Dimethyl glutarate	liq	-205.9			
Sample S		c	-42.51			
2,3-Dimethylhexane liq -60.40 2.17 81.91 2,3-Dimethylhexane g -51.13 4.23 106.11 2,4-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -62.26 0.60 80.96 g -53.21 2.50 104.93 3,3-Dimethylhexane liq -61.58 1.23 81.12 g -52.61 3.17 104.70 3,4-Dimethylhexane liq -60.23 2.03 82.97 g -50.91 4.14 107.15 2,2-Dimethyl-3-hexene liq -34.64 5,5-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,1-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 10methylmaleic anhydride liq -190.2 Dimethylnitramine c -16.9 10methylmaloxalate 14	2,2-Dimethylhexane	liq	-62.63		79.33	
2,3-Dimethylhexane g -51.13 4.23 106.11 2,4-Dimethylhexane liq -61.47 0.89 82.62 g -52.44 2.80 106.51 2,5-Dimethylhexane liq -62.26 0.60 80.96 g -53.21 2.50 104.93 3,3-Dimethylhexane liq -61.58 1.23 81.12 3,4-Dimethylhexane liq -60.23 2.03 82.97 3,4-Dimethyl-3-hexene g -50.91 4.14 107.15 2,2-Dimethyl-3-hexene liq -30.22 7.50.91 4.14 107.15 2,2-Dimethylhydrazine liq -34.64 7.50.91 47.32 39.21 1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 19.0 19.0 40.88 40.88 Dimethylmercury liq 14.0 14.0 14.0 14.0 14.0 14.0 14.0 14		g	-53.71			
2,4-Dimethylhexane liq g -61.47 g 0.89 d 82.62 d 2,5-Dimethylhexane liq -62.26 g 0.60 d 80.96 d 3,3-Dimethylhexane liq -61.58 d 1.23 d 81.12 d 3,4-Dimethylhexane liq -60.23 d 2.03 d 82.97 d 3,4-Dimethyl-3-hexane liq -60.23 d 2.03 d 82.97 d 2,2-Dimethyl-3-hexane liq -30.22 d 4.14 d 107.15 d 2,5-Dimethylhydantoin d c -126.4 d 49.4 d 47.32 d 39.21 d 1,1-Dimethylhydrazine diq diqual diqual diqual diqual diqual diqual dimethyl maleate diqual d		liq	-60.40		81.91	
Section						
2,5-Dimethylhexane liq g -62.26 g 0.60 d 80.96 d 3,3-Dimethylhexane liq -53.21 d 2.50 d 104.93 d 3,4-Dimethylhexane liq -61.58 d 1.23 d 81.12 d 3,4-Dimethylhexane liq -60.23 d 2.03 d 82.97 d 2,2-Dimethyl-3-hexene liq -30.22 d 4.14 d 107.15 d 2,2-Dimethylhydarion liq -34.64 d 4.14 d 107.15 d 5,5-Dimethylhydrazine liq liq 11.8 d 49.4 d 47.32 d 39.21 d 1,1-Dimethylhydrazine liq liq 13.3 d 50.8 d 47.60 d 40.88 d Dimethyl maleate liq liq -168.2 d -139.0 d 14.0 d 40.88 d Dimethylmalonate liq liq 14.0 d -16.9 d 14.0 d 14.0 d 14.0 d Dimethylnitramine c -16.9 d -181.0 d -181.0 d -181.0 d	2,4-Dimethylhexane	liq				
Second						
3,3-Dimethylhexane liq g	2,5-Dimethylhexane	liq				
Section						
3,4-Dimethylhexane liq g -60.23 g 2.03 d 82.97 d 2,2-Dimethyl-3-hexene cis trans liq -30.22 d 107.15 5,5-Dimethylhydantoin cliq 1,1-Dimethylhydrazine liq 1,2-Dimethylhydrazine liq 13.3 d 11,8 d 49.4 d 47.32 d 39.21 d 1,2-Dimethylmaleate Dimethylmaleate Dimethylmaleate Dimethylmaleate Dimethylmaleorathylmale	3,3-Dimethylhexane	liq				
2,2-Dimethyl-3-hexene cis trans liq -30.22 trans liq -34.64 5,5-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 Dimethyl malonate liq -190.2 Dimethyl mercury liq 14.0 Dimethyl malorate liq -181.0 Dimethyl oxalate liq -181.0	0.4.51					
2,2-Dimethyl-3-hexene liq -30.22 trans liq -34.64 5,5-Dimethylhydantoin c -126.4 1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 -139.0	3,4-Dimethylhexane					
cis trans liq liq -30.22 -34.64 5,5-Dimethylhydantoin c -126.4 1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 -139.0 -139.0 -139.0 -139.0 -14.0 -14.0 -14.0 -168.2 -169.0 -169.0 -169.0 -181.0	225: 4.121	g	-50.91	4.14	107.15	
trans liq -34.64 5,5-Dimethylhydantoin c -126.4 1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 -139.0 -139.0 -139.0 -139.0 -14.0 -14.0 -14.0 -14.0 -168.2 -16.9 -16.9 -16.9 -181.0 <td></td> <td>1:-</td> <td>20.22</td> <td></td> <td></td> <td></td>		1:-	20.22			
5,5-Dimethylhydantoin c -126.4 49.4 47.32 39.21 1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 -139.0 -139.0 -139.0 -139.0 -139.0 -14.0 -14.0 -14.0 -16.9 -16.9 -16.9 -16.9 -181.0 -181						
1,1-Dimethylhydrazine liq 11.8 49.4 47.32 39.21 1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 Dimethylmaleic anhydride c -139.0 Dimethyl malonate liq -190.2 Dimethylmercury liq 14.0 Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0						
1,2-Dimethylhydrazine liq 13.3 50.8 47.60 40.88 Dimethyl maleate liq -168.2 -139.0 -13				40.4	47.22	20.21
Dimethyl maleate liq -168.2 Dimethylmaleic anhydride c -139.0 Dimethyl malonate liq -190.2 Dimethylmercury liq 14.0 Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0						
Dimethylmaleic anhydride c -139.0 Dimethyl malonate liq -190.2 Dimethylmercury liq 14.0 Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0				30.8	47.00	40.88
Dimethyl malonate liq -190.2 Dimethylmercury liq 14.0 Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0						
Dimethylmercury liq 14.0 Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0						
Dimethylnitramine c -16.9 Dimethyl oxalate liq -181.0						
Dimethyl oxalate liq -181.0						
2,2-Dimensypermane g 47.27 0.02 93.90 39.07				0.02	93.90	30 67
		5	77.21	0.02	75.70	37.01

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	C_p° , cal \cdot deg ⁻¹ \cdot mol ⁻¹
2,3-Dimethylpentane	g	-47.62	0.16	98.96	39.67
2,4-Dimethylpentane	g	-48.28	0.74	94.80	39.67
3,3-Dimethylpentane	g	-48.17	0.63	95.53	39.67
2,7-Dimethylphenanthrene	c	8.70			
4,5-Dimethylphenanthrene	С	21.26			
9,10-Dimethyl- phenanthrene	С	11.4			
Dimethyl m-phthalate	С	-171			
Dimethyl o-phthalate	liq	-162			
Dimethyl p-phthalate	С	-170			
2,2-Dimethylpropane	g	-39.67	-0.364	73.23	29.07
2,3-Dimethylpyridine	liq	4.62			
2,4-Dimethylpyridine	liq	3.85			
2,5-Dimethylpyridine	liq	4.45			
2,6-Dimethylpyridine	liq	3.02			
3,4-Dimethylpyridine	liq	4.36			
3,5-Dimethylpyridine	liq	5.36			
Dimethyl succinate	liq	-199.6			
1,1-Dimethylsuccinic acid	С	-236.08			
1,2-Dimethylsuccinic acid					
cis	С	-233.6			
trans	С	-235.1			
Dimethyl sulfate	liq	-175.23			
Dimethyl sulfite	liq	-125.07			
Dimethyl sulfone	С	-107.8	-72.3	34.77	
Dimethyl sulfoxide	liq	-48.6	-23.7	45.0	35.2
3,3-Dimethyl-2-thiabutane	liq	-37.49			
2,2-Dimethylthia-	liq	-5.78			
cyclopropane					
2,2-Dimethyl-3-thiapentane	liq	-44.7			
2,4-Dimethyl-3-thiapentane	g	-33.76	6.48	99.30	40.45
2,3-Dinitroaniline	С	-2.8			
2,4-Dinitroaniline	С	-16.3			
2,5-Dinitroaniline	С	-10.6			
2,6-Dinitroaniline	С	-12.1			
3,4-Dinitroaniline	С	-7.8			
3,5-Dinitroaniline	С	-9.3			
2,4-Dinitroanisole	С	-44.6			
2,6-Dinitroanisole	С	-45.2	50.56	51.7	
1,2-Dinitrobenzene	С	2.06	50.56	51.7	
1,3-Dinitrobenzene	С	-4.04	44.13	52.8	
2,4-Dinitrophenol	С	-55.6 50.2			
2,6-Dinitrophenol	С	-50.2			
2,4-Dinitroresorcinol	С	-99.3			

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ},$ kcal·mol $^{-1}$	$\Delta G f^{\circ},$ kcal \cdot mol $^{-1}$	S° , cal \cdot deg ⁻¹ \cdot mol ⁻¹	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
4,6-Dinitroresorcinol	c	-105.1			
2,4-Dinitrotoluene	c	-17.1			
2,6-Dinitrotoluene	c	-12.2			
1,4-Dioxane	liq	-84.47	-44.96	46.67	
	g	-75.30	-43.21	71.65	22.48
1,3-Dioxane	liq	-89.99			
1,4-Dioxatetralin	liq	-60.9			
Dioxindole	c	-76.9			
1,3-Dioxolane	g	-71.1			
Dipentene	liq	-12.1			
<i>N</i> , <i>N</i> -Diphenylacetamide	c	-10.3			
Diphenylamine	c	31.07			
1,4-Diphenylbutadiene					
cis,cis	c	47.51			
trans,trans	c	42.73			
Diphenylbutadiyne	c	123.91			
1,4-Diphenylbutane	c	-2.36			
1,4-Diphenyl-	c	-61.24	1.87	77.6	
1,4-butanedione					
1,4-Diphenyl-2-butene-	c	-27.55	26.64	76.3	
1,4-dione					
Diphenylcarbinol	c	-25.04			
Diphenyl carbonate	c	-95.93	-42.05	66.54	
Diphenyldichlorosilane	liq	-66.5			
Diphenyl disulfide	c	35.8			
Diphenyl disulfone	c	-153.59			
1,1-Diphenylethane	liq	11.7	58.58	80.28	
1,2-Diphenylethane	liq	12.31	63.87	64.6	
1,1-Diphenylethene	liq	41.21			
Diphenyl ether	liq	-3.48	34.47	69.62	
Diphenylethyne	c	74.66			
Diphenylfulvene	c	7.1			
Diphenylmercury	c	66.8			
Diphenylmethane	liq	21.25	66.19	57.2	55.7
Diphenyl sulfide	liq	39.1			
Diphenyl sulfone	c	-53.71			
Diphenyl sulfoxide	c	2.40			
Dipropyl ether	g	-70.00	-25.23	100.98	37.83
Dipropylmercury	liq	-5.0			
Dipropyl sulfate	liq	-205.22			
Dipropyl sulfite	liq	-154.52			
Dipropyl sulfone	liq	-130.94			
Dipropyl sulfoxide	liq	-78.65			
2,3-Dithiabutane	liq	-14.82	1.67	56.26	34.92
5,6-Dithiadecane	g	-37.86	12.87	136.91	55.23

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal \cdot deg ⁻¹ \cdot mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
3,4-Dithiahexane	liq	-28.69	2.28	72.90	
1,3-Dithian-2-thione 4,5-Dithiaoctane <i>N</i> , <i>N</i> -Dithiodiethylamine 1,3-Dithiolan-2-thione Di- <i>p</i> -tolyl sulfone Divinyl ether	c liq liq c c	-3.1 -40.95 -29.1 3.1 -74.32 -9.53	4.56	89.28	
Divinyl sulfone Dodecane Dodecanoic acid	liq liq c	-49.5 -84.16 -185.14	6.71	117.26	89.86
1-Dodecene 1-Dodecyne Dulcitol	g g c	-39.52 -0.01 -321.9	32.96 64.22	147.78 143.98	64.43 63.44
Eicosane Eicosanoic acid (arachidic acid)	g c	-108.93 -241.9	28.04	223.26	110.73
1-Eicosene Ergosterol	g c	-78.93 -188.8	49.03	222.26 39.9	108.15
meso-Erythritol Ethane 1,2-Ethanedithiol	c g liq	-127.56 -20.24 -12.83	-152.12 -7.84	54.76	12.54
Ethanethiol Ethanol	g liq g	-11.02 -66.20 -56.03	-1.12 -41.63 -40.13	70.77 38.49 67.54	17.37 26.76 15.64
Ethoxy radical Ethyl radical Ethyl acetate	g g liq	-6 26.0 -114.49	31 -79.52	59.2 62.0	
Ethyl allyl sulfone Ethylamine	g liq	-105.86 -96.95 -11.00	-78.25 8.91	86.70 68.08	27.16 17.36
N-Ethylaniline Ethylbenzene	g liq liq	0.9 -2.98	45.10 28.61	57.2 60.99	
2-Ethyl-1-butene Ethyl carbamate (urethane)	g g c	7.12 -12.32 -124.4	31.21 19.11	86.15 90.01	30.69 31.92
Ethyl chloride Ethyl crotonate Ethylcyclohexane	g liq liq	-26.83 -100.4 -50.72	-14.46 6.95	65.91 67.14	14.97
1-Ethylcyclohexene Ethylcyclopentane	liq liq	-25.50 -39.08 -30.37	8.92 10.65	67.00 90.42	31.49
Ethyldiethylcarbamate Ethylene	g liq g	-30.37 -141.6 12.50	16.31	52.39	10.24
Ethylene carbonate	С	-138.9			

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Ethylene chlorohydrin	liq	-70.6			
1,2-Ethylenediamine	liq	-15.06		50	
•	aq, 200	-13.32			
Ethylenediaminetetraacetic acid (EDTA)	c	-420.5			
Ethylenediammonium chloride	с	-122.7			
	aq, 5000	-115.92			
Ethylene glycol	liq	-108.70	-77.25	39.9	35.8
(2,1-ethanediol)	1				
(, ,	g	-93.05	-72.77	77.33	23.20
	aq, 1	-109.01			
Ethyleneimine (azirane)	g	29.50	42.54	59.90	12.55
Ethylene oxide	g	-12.58	-3.13	57.94	11.54
2-Ethyl-1-hexanal	liq	-83.30			
2-Ethyl-2-hexanal	liq	-62.44			
3-Ethylhexane	liq	-59.88	1.79	84.95	
Ethylidenecyclohexane	liq	-21.19			
Ethyl isovalerate	liq	-136.5			
Ethyllithium	c	-14.0			
Ethylmercury bromide	c	-25.7			
Ethylmercury chloride	c	-33.7			
Ethylmercury iodide	c	-15.7			
Ethyl methyl ether	g	-51.73	-28.12	74.24	21.45
Ethyl nitrate	g	-36.80	-8.81	83.25	23.27
Ethyl nitrite	g	-24.9		24.74	23.71
3-Ethylpentane	g	-45.33	2.63	98.35	39.67
Ethyl pentanoate	liq	-132.2			
Ethyl peroxyl radical	g	(-2)			
2-Ethylphenol	c	-49.91			
3-Ethylphenol	c	-51.21			
4-Ethylphenol	c	-53.63			
Ethylphosphonic acid	С	-251.3			
Ethyl propanoate	liq	-122.16	-79.16		
2-Ethylpyridine	liq	-1.2			
Ethylsuccinic acid	c	-236.4			
Ethyl thioacetate	liq	-64.01			
Ethyl β -vinylacrylate	liq	-80.8			
Ethyl vinyl ether	g	-33.63			
Ethynylbenzene (phenylacetylene)	g	78.22	86.46	76.88	27.46
Fluoranthene	c	45.75	82.60	55.09	
Fluoroacetamide	c	-118.7			
Fluoroacetic acid	c	-164.5			
Fluorobenzene	g	-27.86	-16.50	72.33	22.57
2-Fluorobenzoic acid	c	-135.67			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
3-Fluorobenzoic acid	С	-139.13			
4-Fluorobenzoic acid	c	-140.00			
Fluoroethane	g	-62.90	-50.44	63.34	14.21
2-Fluoroethanol	liq	-111.3			
Fluoromethane	g	-56.80	-51.09	53.25	8.96
1-Fluoropropane	g	-67.20	-47.87	72.71	19.75
2-Fluoropropane	g	-69.00	-48.81	69.82	19.60
4-Fluorotoluene	liq	-44.80	-19.06	56.67	
Fluorotrinitromethane	liq	-52.8			
Formaldehyde	g	-27.70	-26.27	52.29	8.46
unhydrolyzed	aq	-35.9	-31.02		
Formamide	liq	-60.7			
	g	-44.5	-33.71	59.41	10.84
Formanilide	c	-36.2			
Formic acid	liq	-101.51	-86.38	30.82	23.67
	g	-90.49	-83.89	59.45	10.81
Ionized; std state, $m = 1$	aq	-101.71	-83.9	22	-21.0
Nonionized; std state,	aq	-101.68	-89.0	39	
m = 1	_				
Dimer	g	-195.08			
Formyl					
HCO	g	10.4	6.76	53.66	8.27
HCO ⁺	g	204	201	48.3	8.62
Formyl fluoride	g	-90	-88	59.0	9.66
N-Formyl-DL-leucine	c	-222.1			
Formyl urea	c	-118			
β -D-Fructose	С	-302.2			
D-Fucose	С	-262.7			
Fumaric acid	С	-193.84	-156.70	39.7	
Fumaronitrile	С	64.11			
Furan	g	-8.23	0.21	63.86	15.64
Furfural	liq	-47.8			
Furfuryl alcohol	liq	-66.05	-36.85	51.50	
2-Furoic acid	С	-119.12			
(pyromucic acid)		100 5			
Furylacrylic acid	c	-109.7			
Furylethylene	liq	-2.5			
D-Galactonic acid	c	-384.8			
D-Galactose	c	-304.1	-219.60	49.1	
D-Glucaric acid-	c	-343.2			
1,4-lactone					
D-Glucaric acid-	с	-343.6			
3,6-lactone					
D-Gluconic acid	с	-379.3			
D-Gluconic acid-δ-	С	-300.3			
lactone					

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		$\Delta H f^{\circ}$,	$\Delta G\!f^{\circ},$	S° , cal $\cdot \deg^{-1} \cdot$	C_p° , cal $\cdot \deg^{-1} \cdot$
Substance	State	$kcal \cdot mol^{-1}$	kcal·mol ⁻¹	mol ⁻¹	mol ⁻¹
D-Glucose					
α	c	-304.26	-217.6	50.7	
β	c	-302.76			
D-Glutamic acid	c	-240.19	-173.87	45.7	
L-Glutamic acid	c	-241.32	-174.78	44.98	
L-Glutamine	c	-197.3			
Glutaric acid	С	-229.44			
Glyceraldehyde	liq	-143			
Glycerol	liq	-159.76	-114.01	48.87	35.9
Glyceryl-1-acetate	liq	-217.5			
Glyceryl-l-benzoate	c c	-185.80			
Glyceryl-2-benzoate	c	-184.71			
Glyceryl-1-caprate	c	-265.05			
Glyceryl-2-caprate	c	-261.90			
Glyceryl-1,3-diacetate	liq	-268.2			
Glyceryl-1-laurate	c 1	-277.46			
Glyceryl-2-laurate	c	-275.48			
Glyceryl-2-myristate	c	-292.31			
Glyceryl-1-palmitate	c	-306.28			
Glyceryl-1-stearate	c	-319.64			
Glyceryl triacetate	liq	-318.3			
Glyceryl trilaurate	c	-489			
Glyceryl trimyristate	c	-520			
Glyceryl trinitrate	lig	-88.6			
Glycine	c	-126.22	-88.09	24.74	23.71
Ionized; std state, $m = 1$	aq	-112.28	-75.28	26.54	20171
Nonionized; std state,	aq	-122.85	-88.62	37.84	
m=1	aq	122.03	00.02	37.04	
MH₃+CH₂COOH;	aq	-123.78	-91.82	45.46	
std state, $m = 1$	aq	123.70	71.02	45.40	
Glycol acetal	liq	-91.1			
Glycolic acid	c	-158.6			
(hydroxyacetic acid)		130.0			
Glycylglycine	c	-178.51	-117.25	45.4	
Glycylphenylalanine	c	-163.9	117.23	43.4	
Glycylvaline	c	-200.0			
Glyoxal		-50.66			
Glyoxime	g c	-30.66 -21.63			
*					
Glyoxylic acid Guanidine	С	-199.7			
Guanidine carbonate	c	-13.39 -232.10	_122.22	70.6	61.87
	С	-232.10	-133.23	/0.0	01.8/
Guanidine nitrate	С	-92.5			
Guanidine sulfate Guanine	С	-288.0	11 22	38.3	
Guaiiille	С	-43.72	11.33	36.3	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

	ı			I	
Substance	State	$\Delta H f^{\circ}$, keal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	C_p° , cal $\cdot \deg^{-1} \cdot \gcd^{-1}$
Guanylurea nitrate	c	-102.1			
Heptadecane Heptadecanoic acid	g c	-94.15 -220.9	22.01	195.33	94.33
1-Heptadecene 1-Heptanal	g g	-64.15 -63.10	43.00 -20.71	194.33 110.34	91.76 40.89
Heptane Heptanedioic acid	liq g	-53.63 -44.88	0.42 1.91	77.92 102.27	53.76 39.67
1-Heptanethiol	g liq	-35.76 -145.75	8.65	117.89	44.68
Heptanoic acid (enanthic acid)	c	-241.75			
1-Heptanol	liq g	-95.8 -79.3	-34.0 -28.9	76.5 114.8	66.5 42.7
1-Heptene	liq	-23.41 -14.89	21.22 22.90	78.31 101.24	50.62 37.10
1-Heptyne Hexachlorobenzene	g	24.62	54.18	97.44 62.20	36.11 48.11
	c g	-31.30 -8.10	0.25 10.56	105.45	41.40
Hexachloroethane Hexadecafluoroethyl- cyclohexane	g liq	-33.20 -799.1	-13.13	95.30	32.68
Hexadecafluoroheptane	liq g	-817.6 -808.9	-739.24 -737.87	134.28 158.88	
Hexadecane Hexadecanoic acid (palmitic acid)	g c	-89.23 -213.3	20.00 -75.54	186.02 108.12	88.86
1-Hexadecanol (cetyl alcohol)	c, II	-163.4	-23.6	108.0	104.8
1-Hexadecene Hexafluorobenzene	liq g liq	-151.86 -59.23 -237.27	$ \begin{array}{r} -23.08 \\ 40.99 \\ -211.43 \end{array} $	145.0 185.02 66.90	86.29 52.96
Hexafluoroethane Hexahydroindane	gg gg	-228.64 -320.90	-210.18 -300.15	91.59 79.30	37.43 25.43
cis trans	g g	-30.4 -31.4			
Hexamethyldisiloxane	c liq	-39.19 -194.7	28.06 -129.5	71.66 103.69	61.5 74.42
Hexamethylenetetramine (urotropine)	c liq	30.0 -18.7	103.92 28.65	39.05 73.28	25.42
Hexanal Hexanamide	g c	-59.37 -101.48	-23.93	101.07	35.43
Hexane	liq g	-47.52 -39.96	-0.91 -0.06	70.76 92.83	45.2 34.20
1-Hexanethiol Hexanoic acid	g liq	-30.83 -139.71	6.65	108.58	39.21

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	ΔGf° , kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	C_p° , cal · deg ⁻¹ · mol ⁻¹
1-Hexanol	liq	-90.7	-36.4	69.2	56.6
	g	-75.9	-32.4	105.5	37.2
1-Hexene	liq	-17.30	19.93	70.55	43.81
ТПОЛОПО	1 ^	-9.96	20.90	91.93	31.63
2-Hexene	g	7.70	20.50	71.73	31.03
cis	g	-12.51	18.22	92.37	30.04
trans	_	-12.27	18.27	90.97	31.64
3-Hexene	g	12.27	16.27	90.97	31.04
cis		-11.38	19.84	90.73	29.55
	g				
trans	g	-13.01	18.55	89.59	31.75
1-Hexyne	g	29.55	52.24	88.13	30.65
Hippuric acid	c	-145.63	-88.33	57.2	
(benzoylglycine)					
Hydantoic acid	С	-179			
Hydantoin	С	-107.2			
Hydrazobenzene	c	52.9			
Hydroquinone	c	-87.08	-49.48	33.5	33.9
Hydrosorbic acid	liq	-110.2			
Hydroxyacetic acid	c	-158.6			
o-Hydroxybenzoic acid	c	-140.64	-100.7	42.6	38.03
m-Hydroxybenzoic acid	c	-139.8	-99.74	42.3	37.59
<i>p</i> -Hydroxybenzoic acid	c	-139.7	-99.55	42.0	37.08
β -Hydroxybutyric acid	liq	-162.3			
Hydroxyisobutyric acid	c	-177.9			
L-Hydroxyproline	c	-158.1			
8-Hydroxyquinoline	c	-19.9			
Hypoxanthene	c	-26.47	18.39	34.8	
(6-oxypurine)					
Imidazole		145			
	c	14.5	26.04	56.01	45.47
Indane	liq	2.56	36.04	56.01	45.47
Indene	liq	26.39	52.00	51.19	44.68
Indole	С	29.8	44.00	5 0.04	24.00
Iodobenzene	g	38.85	44.88	79.84	24.08
2-Iodobenzoic acid	С	-72.2 -75.7			
3-Iodobenzoic acid	c	-75.7			
4-Iodobenzoic acid	c	-75.5			
Iodocyclohexane	liq	-23.5			
Iodoethane	liq	-9.6	3.5	50.6	27.5
	g	-2.00	5.10	70.82	15.76
Iodomethane	liq	-3.29	3.61	38.9	
	g	3.29	3.72	60.64	10.54
2-Iodo-2-methylpropane	g	-17.60	5.65	81.79	28.27
1-Iodonaphthalene	liq	38.6			
2-Iodonaphthalene	c	34.5			
2-Iodophenol	c	-22.9			
	_				

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

	1		I	I	
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ},$ kcal·mol $^{-1}$	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
3-Iodophenol	c	-22.6			
4-Iodophenol	c	-22.8			
1-Iodopropane	g	-7.30	6.68	80.32	21.48
2-Iodopropane	g	-10.00	4.80	77.55	21.53
3-Iodopropene	liq	13.7	1.00	77.55	21.33
(allyl iodide)	nq	13.7			
3-Iodopropionic acid	c	-109.9			
2-Iodotoluene	liq	18.7			
3-Iodotoluene	liq	18.9			
4-Iodotoluene	liq	16.1			
Isatin	c	-62.7			
Isobutylbenzene	liq	-16.68			
Isobutyl dichloracetate	liq	-132.4			
Isobutyl phenyl ketone	liq	-52.63			
Isobutyl trichloroacetate	liq	-132.4			
Isobutyronitrile	g	6.07	24.76	74.88	23.04
L-Isoleucine	c	-151.8	-82.97	49.71	45.00
Isopropenyl acetate	liq	-92.31			
Isopropyl radical	g	17.6			
Isopropyl acetate	liq	-124.01			
lsopropylbenzene	liq	-9.85	29.70	66.87	
(cumene)	g	0.94	32.74	92.87	36.26
Isopropyl nitrate	g	-45.65	-9.72	89.20	28.84
Isopropyl thiolacetate	liq	-71.26			
Isopropyl trichloroacetate	liq	-128.2			
Isoquinoline	c	37.9			
L-Isoserine	С	-177.8			
Isothiocyanic acid	g	30.50	26.98	59.28	11.09
Itaconic acid	С	-201.06			
Ketene	g	-14.60	-14.41	57.79	12.37
α -Ketoglutaric acid	c	-245.35			
D-Lactic acid	c	-165.88		34.3	
L-Lactic acid	c	-165.89	-124.98	34.00	
	liq	-161.2	-123.84	45.9	
β -Lactose	c	-534.1	-374.52	92.3	
Lauric acid (dodecanoic acid)	c	-185.14			
D-Leucine	c	-152.36	-82.97	49.71	
L-Leucine	c	-154.6	-82.76	50.62	48.03
DL-Leucine	c	-153.14	-83.54	49.5	10.03
DL-Leucylglycine	c	-205.7	-112.14	67.2	
Leucylglycylglycine	c	-259.6		02	
Levulinic acid	c	-166.6			
Levulinic lactone	liq	-76.2			
(+)-Limonene	liq	-13.0			
DL-Lysine	c	-162.2			

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		ΔHf° ,	$\Delta G f^{\circ}$,	S° , cal \cdot deg ⁻¹ \cdot	C_p° , cal $\cdot \deg^{-1} \cdot$
Substance	State	$kcal \cdot mol^{-1}$	$\frac{\Delta O_J}{\text{kcal} \cdot \text{mol}^{-1}}$	mol ⁻¹	mol ⁻¹
	State	11011	nour mor	11101	11101
Maleic acid	С	-188.94	-149.40	38.1	32.36
Maleic anhydride	c	-112.08			
L-Malic acid	С	-263.78	-211.45		
DL-Malic acid	С	-264.27			
Malonamide	С	-130.5			
Malonic acid	С	-212.96			
Malonic diamide	С	-130.52			
Malononitrile	С	44.6			
Maltose	С	-530.8	-412.60		
L-Mandelic acid	С	-138.8			
D-Mannitol	С	-139.61	-225.20	57.0	
D-Mannose	С	-301.9			
Melamine	С	-17.3	44.10	35.63	
(triaminotraizine)					
Melezitose	С	-815			
2-Mercaptopropionic acid	liq	-111.9	-82.19	54.70	
Mesaconic acid	С	-197			
Mesoxalic acid	С	-290.7			
2,2-Metacyclophane	g	40.8			
Methane	g	-17.89	-12.15	44.52	8.54
Methanethiol	g	-5.49	-2.37	60.96	12.01
(methyl mercaptan)					
Methanol	liq	-57.13	-39.87	30.41	19.40
	g	-48.06	-38.82	57.29	10.49
Std state, $m = 1$	aq	-58.78			
L-Methionine	С	-180.4	-120.88	55.32	
Methoxyl radical	g	(2)			
2-Methoxybenzaldehyde	С	-63.7			
3-Methoxybenzaldehyde	liq	-66.0			
4-Methoxybenzaldehyde	liq	-63.9			
Methoxybenzene (anisole)	g	-17.3			
Methoxymethyl radical	g	(-4)			
2-Methoxytetrahydropyran	liq	-105.7			
5-Methoxytetrazole	С	16.6			
Methyl (CH ₃) radical	g	34.82	35.35	46.38	9.25
Methyl acetate	liq	-106.4			
Methyl acrylate	g	-70.10	-56.78		
Methyl allantoin (pyvurile)	С	-177.0			
Methyl allyl sulfone	liq	-91.95			
Methylamido radical	g	35			
(CH ₃ NH)		5.50	7.71	57.00	11.07
Methylamine	g	-5.50	7.71	57.98	11.97
Std state, $m = 1$	aq	-16.77	4.94	29.5	
Methylaminolithium	C Lia	-22.92			
<i>N</i> -Methylaniline	liq	7.7			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Methyl benzoate	liq	-79.8			
Methyl benzyl sulfone	c	-88.65			
2-Methylbiphenyl	liq	25.8			
3-Methylbiphenyl	liq	20.4			
4-Methylbiphenyl	c	13.2			
2-Methyl-1,3-butadiene (isoprene)	g	18.10	34.86	75.44	25.00
3-Methyl-1,2-butadiene	g	31.00	47.47	76.40	25.20
2-Methylbutane	g	-36.92	-3.54	82.12	28.39
3-Methyl-1-butanethiol	g	-27.44			
2-Methyl-2-butanethiol	liq	-38.90	0.56	69.34	
	g	-30.36	2.20	92.48	34.30
2-Methyl-1-butanol	liq	-85.2			52.6
3-Methyl-1-butanol	liq	-85.2			50.3
2-Methyl-2-butanol	liq	-90.7	-41.9	54.8	59.2
	g	-78.8	-39.5	86.7	
3-Methyl-2-butanol	liq	-87.5	1.5.00	04.45	55.5
2-Methyl-1-butene	g	-8.68	15.68	81.15	26.28
3-Methyl-1-butene	g	-6.92	17.87	79.70	28.35
2-Methyl-2-butene	g	-10.17	14.26	80.92	25.10
Methyl butyl sulfone	liq	-128.00			
Methyl <i>tert</i> -butyl sulfone	С	-132.8	40.12	76.23	25.02
3-Methyl-1-butyne Methyl caprate	g liq	32.60 -153.07	49.12	70.23	25.02
Methyl caproate	liq	-133.07 -129.10			
(methyl hexanoate)	nq	129.10			
N-Methylcaprolactam	liq	-73.3			
5-Methylcaprolactam	c	-86.9			
7-Methylcaprolactam	c	-86.5			
Methyl caprylate	liq	-141.07			
(methyl octanoate)	119	11107			
Methyl chloride	g	-19.59	-13.97	55.97	9.74
Methyl crotonate	liq	-91.5			
Methylcyclohexane	liq	-45.45	4.86	59.26	
• •	g	-36.99	6.52	82.06	32.27
2-Methylcyclohexanol					
cis	liq	-93.3			
trans	liq	-99.4			
3-Methylcyclohexanol					
cis	liq	-99.5			
trans	liq	-94.3			
4-Methylcyclohexanol					
cis	liq	-98.8			
trans	liq	-103.6			
2-Methylcyclohexanone	liq	-68.8			
Methylcyclopentane	g	-25.50	8.55	81.24	26.24

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		ATTCO	A G 69	S°,	C_p° ,
Substance	State	Δ <i>Hf</i> °, kcal⋅mol ⁻¹	ΔGf° , kcal·mol ⁻¹	cal · deg ⁻¹ · mol ⁻¹	cal·deg ⁻¹ ·mol ⁻¹
1-Methylcyclopentanol	liq	-82.3			
2-Methylcyclopentanone	liq	-63.4			
1-Methylcyclopentene	g	-1.30	24.41	78.00	24.10
3-Methylcyclopentene	g	2.07	27.48	79.00	23.90
4-Methylcyclopentene	g	3.53	29.06	78.60	23.90
Methyldichlorosilane	liq	-105.9			
2-Methyl-1,3-dioxane	liq	-104.60			
4-Methyl-1,3-dioxane	liq	-99.80			
<i>N</i> -Methyldiphenylamine	liq	28.8			
4-Methyldiphenylamine	С	11.7			
Methylene	g	92.35	88.25	46.32	8.27
2-Methylenecyclohexanol	liq	-66.3			
2-Methylenecyclopentanol		11.2			
β -Methylene- β -propiolactone (diketene)	liq	-55.72			
Methylene sulfate	С	-164.6			
1-Methyl-2-ethylbenzene	g	0.29	31.33	95.42	37.74
1-Methyl-3-ethylbenzene	g	-0.46	30.22	96.60	36.38
1-Methyl-4-ethylbenzene	g	-0.78	30.28	95.34	36.22
2-Methyl-3-ethylpentane	liq	-59.69	3.03	81.41	
234 4 12 4 1	g	-50.48	5.08	105.43	
3-Methyl-3-ethylpentane	liq	-60.46	2.69 4.76	79.97 103.48	
2-Methyl-3-ethyl-1- pentene	g g	-51.28 -23.97	4.70	103.46	
Methyl ethyl sulfite	liq	-135.55			
Methyl ethyl sulfone	c	-116.17			
Methyl formate	lig	-90.60	-71.53	29	
, ,	g	-83.70	-71.03	72.00	15.90
Methylglyoxal	g	-64.8			
Methylglyoxime	c	-30.3			
2-Methylheptane	liq	-60.98	0.92	84.16	
	g	-51.50	3.05	108.81	
3-Methylheptane	liq	-60.34	1.12	85.66	
	g	-50.82	3.28	110.32	
4-Methylheptane	liq	-60.17	1.87	83.72	
	g	-50.69	4.00	108.35	
Methyl heptanoate	liq	-135.54			
2-Methylhexane	liq	-54.93	-0.69	77.28	53.28
	g	-46.59	0.77	100.38	39.67
3-Methylhexane	liq	-54.35	-0.39	78.23	
	g	-45.96	1.10	101.37	39.67
Methyl hexanoate	liq	-129.11			
5-Methylhydantoin	c	-116.3	12.0	20.55	22.5
Methylhydrazine	liq	12.9	43.0	39.66	32.25
	g	22.55	44.66	66.61	17.0

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	C_p° , $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot \operatorname{mol}^{-1}$
Methylidyne					
CH	g	142.00	134.02	43.72	6.97
CH ⁺	g	388.8	380.1	41.00	6.97
α -Methylindole	c	14.5			
Methyl isocyanide	g	35.6	39.6	58.99	12.65
1-Methyl-2-isopropyl- benzene (<i>o</i> -cymene)	liq	-18.19			
1-Methyl-3-isopropyl- benzene	liq	-18.69			
Methyl isopropyl ether	g	-60.24	-28.89	80.86	26.55
Methyl isopropyl ketone	g	-62.76			
Methyl isopropyl sulfone	liq	-120.44			
Methyl isothiocyanate (CH ₃ NCS)	g	31.3	34.5	69.29	15.65
3-Methylisoxazole	liq	-5.0			
5-Methylisoxazole	liq	-6.4			
Methyl laurate	liq	-165.66			
Methylmercury bromide	c	-20.6			
Methylmercury chloride	c	-27.8			
Methylmercury iodide	c	-10.4			
Methyl myristate	liq	-177.80			
1-Methylnaphthalene	liq	13.43	46.26	60.90	53.63
2-Methylnaphthalene	c	10.72	46.03	52.58	46.84
Methyl nitrate	liq	-38.0	-10.4	51.9	37.6
	g	-29.8	-9.4	76.1	
Methyl nitrite	g	-15.30	0.24	67.95	15.11
Methyl oleate	liq	-174.2			
Methyl pelargonate	liq	-147.29			
2-Methylpentane	g	-41.66	-1.20	90.95	34.46
3-Methylpentane	g	-41.02	-0.51	90.77	34.20
Methyl pentanoate	liq	-122.90	10.55	01.24	22.41
2-Methyl-1-pentene	g	-12.49	18.55	91.34	32.41
3-Methyl-1-pentene	g	-10.76	20.66	90.06	34.04
4-Methyl-1-pentene	g	-10.54	21.52	87.89	30.23
2-Methyl-2-pentene	g	-14.28	17.02	90.45	30.26
3-Methyl-2-pentene		12.00	17.50	00.45	20.26
cis	g	-13.80	17.50	90.45	30.26
trans 4 Mathyl 2 pantana	g	-14.02	17.04	91.26	30.26
4-Methyl-2-pentene <i>cis</i>		12.02	19.63	89.23	31.92
trans	g	-12.03 -12.99	19.03	88.02	33.80
Methyl pentanoate	g liq	-122.89	17.03	00.02	33.00
Methyl phenyl sulfone	c	-82.49			
(2-Methyl phenol)		-30.74	-8.86	85.47	31.15
(2 Monty) phonon	g	30.74	0.00	05.47	51.15

5.30 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

			I	I	1
				S°,	C_p° ,
		ΔHf° ,	$\Delta G f^{\circ}$,	$cal \cdot deg^{-1} \cdot$	cal · deg ⁻¹ ·
Substance	State	kcal⋅mol ⁻¹	kcal·mol ⁻¹	mol^{-1}	mol^{-1}
-					
(3-Methyl phenol)	g	-31.63	-9.69	85.27	29.27
(4-Methyl phenol)	g	-29.97	-7.38	83.09	29.75
Methylphosphonic acid	c	-252	7.50	03.07	27.13
2-Methylpropanal	g	-52.25			
2-Methylpropane	_	-32.15	-4.99	70.42	23.14
2-Methyl-	g liq	-32.00	4.55	70.42	23.14
1,2-propanediamine	nq	32.00			
2-Methyl-1-propanethiol		-23.24	1.33	86.73	28.28
	g	-25.24 -26.17	0.17	80.79	28.26
2-Methyl-2-propanethiol	g				
2-Methyl-1-propanol	g 1: -	-67.69	-39.99	85.81	26.6
2-Methyl-2-propanol	liq	-85.86	-44.14	46.10	52.61
236.4.1	g	-74.67	-42.46	77.98	27.10
2-Methylpropene	g	-4.04	13.88	70.17	21.30
Methyl propyl ether	g	-56.82	-26.27	83.52	26.89
7-Methylpurine	c	51.3	20.00	52.05	27.04
2-Methylpyridine	liq	13.83	39.80	52.07	37.86
(2-picoline)		2405	40.00	55 60	22.00
	g	24.05	42.32	77.68	23.90
3-Methylpyridine	liq	15.57	41.16	51.70	37.93
4-Methylpyridine	liq	13.58			
N-Methylpyrrolidone	liq	-62.64			
Methyl salicylate	liq	-127.1			
α -Methylstyrene	liq	16.8			
0.34 4 1	g	27.00	49.84	91.70	34.70
β -Methylstyrene	_	20.00	51.04	01.70	34.70
cis	g	29.00	51.84	91.70	
trans	g	28.00	51.08	90.90	34.90
Methylsuccinic acid	c	-229.02	2.21	05.07	20.00
3-Methyl-2-thiabutane	g	-21.61	3.21	85.87	28.00
2-Methylthiacyclopentane	g 1: -	-15.12 -37.3			
2-Methyl-3-thiapentane	liq	16.31			
4-Methylthiazole	liq	10.75	27.25	52.22	29.43
2-Methylthiophene	liq	10.75	27.35 27.00	52.22	29.43
3-Methylthiophene 4-Methyluracil	liq		27.00	32.19	29.36
-	C 1: -	-109.2			
Methyl valerate	liq	-122.89			
(methyl pentanoate) Morphine monohydrate		-170.1			
Mucic acid	С	-423			
Murexide	c				
	C 1: a	-289.7 3.5			
Myrcene	liq				
Myristic acid (tetradecanoic acid)	С	-199.21			
· ·					
Naphthalene	С	18.0	48.05	39.89	
137 1.1 1	g	35.6	53.44	80.22	31.68
1-Naphthol	g	-5.1			
·					

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal \cdot deg ⁻¹ \cdot mol ⁻¹	C_p° , $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot \operatorname{mol}^{-1}$
2-Naphthol	g	-10.1			
1,4-Naphthoquinone	c	-43.83			
1-Naphthyl acetate	c	-68.89			
2-Naphthyl acetate	c	-72.72			
1-Naphthylamine	c	16.2			
2-Naphthylamine	c	14.4			
Narceine dihydrate	c	-421.2			
Narcotine	c	-210.9			
Nicotine	liq	9.4			
Nitrilotriacetic acid	c		-312.5		
2-Nitroaniline	c	-3.45	42.60	42.1	39.3
3-Nitroaniline	c	-4.46	41.60	42.1	40.2
4-Nitroaniline	c	-9.91	36.10	42.1	40.4
Nitrobenzene	liq	3.80	34.95	53.6	44.4
2-Nitrobenzoic acid	c	-94.25	-46.95	49.8	
3-Nitrobenzoic acid	c	-100.25	-52.71	49.0	
4-Nitrobenzoic acid	c	-101.25	-53.07	50.2	43.3
3-Nitrobiphenyl	c	15.6			
4-Nitrobiphenyl	c	9.7			
1-Nitrobutane	g	-34.40	2.42	94.28	29.85
2-Nitrobutane	g	-39.10	-1.49	91.62	29.51
3-Nitro-2-butanol	liq	-93.2			
2-Nitrodiphenylamine	c	15.4			
Nitroethane	g	-24.4	-1.17	75.39	18.69
aci form	aq	-30.7			
nitro form	aq	-32			
2-Nitroethanol	liq	-83.8			
Nitroguanidine	c	-22.1			
Nitromethane	liq	-27.03	-3.47	41.05	25.33
	g	-17.86	-1.66	65.73	13.70
1-Nitronaphthalene	С	10.2		0.5.00	24.44
1-Nitropropane	g	-30.00	0.08	85.00	24.41
2-Nitropropane	g	-33.21	-3.06	83.10	24.26
4-Nitrosodiphenylamine	С	50.9	26.02	212.05	105.06
Nonadecane 1-Nonadecene	g	-104.00	26.03	213.95	105.26
1-Nonadecene 1-Nonanal	g	-74.00	47.02 -17.91	212.95	102.69 51.82
Nonane	g	-74.16 -65.84	2.81	128.97 94.09	31.62
Nonane	liq		5.93	120.86	50.60
1-Nonanethiol	g	-54.74 -45.61	3.93 12.67	136.51	55.61
Nonanoic acid	g lia	-43.61 -157.68	12.07	130.31	33.01
1-Nonanol	liq liq	-137.68 -109.2	-32.4	91.3	67.50
1-Nonene	1 *	-109.2 -24.74	26.93	119.86	48.03
	g				
Octadecane	g	-99.08	24.02	204.64	99.80
Octadecanoic acid	С	-226.5			
	1	1		I	<u> </u>

5.32 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		A 7700	A G (0)	S°,	C_p° ,
Substance	State	ΔHf° , kcal·mol ⁻¹	ΔGf° , kcal·mol ⁻¹	cal · deg ⁻¹ · mol ⁻¹	cal·deg ⁻¹ ·mol ⁻¹
1-Octadecene	g	-69.08	45.01	203.64	97.22
Octafluorocyclobutane	g	-365.20	-334.33	95.69	37.32
1-Octanal	g	-69.23	-19.91	119.66	46.36
Octanamide	c	-113.1			
Octane	liq	-59.74	1.77	85.50	45.14
	g	-49.82	3.92	111.55	45.14
1-Octanethiol	g	-40.68	10.67	127.20	50.14
Octanoic acid	liq	-151.93			
(caprylic acid)	1				
1-Octanol	liq	-101.6	-34.2	90.2	77.7
2-Octanone	liq	-91.9	-33.54	89.35	65.31
1-Octene	liq	-29.52	22.49	86.15	57.65
	g	-19.82	24.91	110.55	42.56
1-Octyne	g	19.70	56.26	106.75	41.58
Oleic acid	c	-187.2			
DL-Ornithine	c	-156.0			
Oxacyclobutane	g	-19.25	-2.33	65.46	
(trimethylene oxide)					
Oxalic acid	c	-197.7	-166.8	28.7	
Std state, $m = 1$	aq	-197.2	-161.1	10.9	
Oxalic acid dihydrate	c	-341.0			
Oxalyl chloride	liq	-85.6			
Oxamic acid	c	-160.4			
Oxamide	c	-123.0	-81.9	28.2	
Oxindole	c	-41.2			
8-Oxypurine	c	-15.4			
Palmitic acid	c	-213.10			
(hexadecanoic acid)		213.10			
Papaverine Papaverine	c	-120.2			
Parabanic acid	c	-138.0			
[1,8]-Paracyclophane	c	-19.6			
[2,2]-Paracyclophane	g	59.9			
[6,6]-Paracyclophane	c	-46.1			
Paraldehyde	liq	-164.2			
Pentachloroethane	g	-34.8	-16.79	91.17	28.22
Pentachlorofluoroethane	g	-75.8	-55.93	93.54	
Pentachlorophenol	c	-70.6	-34.44	60.21	48.27
Pentadecane	g	-84.31	17.98	176.71	83.40
1-Pentadecene	g	-54.31	38.97	175.71	80.82
1-Pentadecyne	g	-14.78	70.25	171.91	79.84
1,2-Pentadiene	g	34.80	50.29	79.70	25.20
1,3-Pentadiene					
cis	g	18.70	34.84	77.50	22.60
trans	g	18.60	35.07	76.40	24.70
1,4-Pentadiene	g	25.20	40.69	79.70	25.10

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			ı			
Substance State kcal·mol ⁻¹ kcal·mol ⁻¹ mol ⁻¹ mol ⁻¹ 2,3-Pentadiene g 33.10 49.21 77.60 24.20 Pentacrythritol c -220.0 -146.73 47.34 45.51 Pentafluorobenzoic acid c -220.34 -264.00 79.76 22.88 Pentafluorophenol c -244.86 -264.00 79.76 22.88 Pentafluorophenol c -244.86 -25.88 91.53 29.96 Pentamethylbenzoic acid c -128.13 -25.88 91.53 29.96 Pentamanide c -90.70 95.1 28.7 Pentamenin-1,5-dithiol liq -30.99 95.1 28.73 Pentamenin-1,5-dithiol liq -			A 77CO	A C (°)		C_p° ,
Pentaerythritol C	Substance	State				mol ⁻¹
Pentaerythritol tetranitrate Pentafluorobenzoic acid Pentafluoropthane c -128.8 -296.34 -246.00 79.76 22.88 Pentafluoropthane g -264.00 -246.00 79.76 22.88 Pentafluorophenol c -244.86 -244.86 70.22 51.74 Pentamethylbenzoic acid c -128.13 25.64 70.22 51.74 Pentananide c -128.13 25.64 70.22 51.74 Pentanenthylbenzoic acid c -90.70 -25.88 91.53 29.96 Pentanenthylbenzoic acid liq -101.33 -25.88 91.53 29.96 Pentanenthylbenzoic acid liq -101.33 -25.88 91.53 29.96 Pentanentanenthiol liq -101.33 -25.88 91.53 29.96 Pentanentanenthiol liq -30.97 95.1 28.7 Pentanenthylbenzoic acid liq -35.72 2.28 74.18 Pentanenthylbenzoic acid liq -85.0 -38.3 62.0 <	2,3-Pentadiene	g	33.10	49.21	77.60	24.20
Pentafluorobenzoic acid c -296.34 -246.00 79.76 22.88 Pentafluorophenol c -244.86 -244.86 70.22 51.74 Pentamethylbenzene liq -32.33 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 25.64 70.22 51.74 Pentamal g -54.45 -25.88 91.53 29.96 Pentamal g -54.45 -25.88 91.53 29.96 Pentanid liq -101.33 29.96 29.96 Pentanid liq -30.99 95.1 28.7 Pentanic g -35.00 -2.00 83.40 28.73 1-Pentanethiol liq -33.72 2.28 74.18 74.18 Pentamethylez liq -85.0 -38.3 62.0 49.8 2-Pentanel liq -85.0 -38.3 <td< td=""><td></td><td>c</td><td>-220.0</td><td>-146.73</td><td>47.34</td><td>45.51</td></td<>		c	-220.0	-146.73	47.34	45.51
Pentafluoroethane g -264.00 -246.00 79.76 22.88 Pentafluorophenol c -244.86 5 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 -25.88 91.53 29.96 Pentamethylbenzoic acid liq -101.33 -25.88 91.53 29.96 Pentamethylbenzoic acid liq -101.33 -25.88 91.53 29.96 Pentaninide c -90.047 95.1 28.7 Pentanidide g -00.47 95.1 28.7 Pentanidide liq -30.99 95.1 28.7 Pentanidide liq -35.72 2.28 74.18 74.18 Pentanethiol liq -35.72 2.28 74.18 74.18 Pentanethiol liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 38.9<	Pentaerythritol tetranitrate	c	-128.8			
Pentafluorophenol c -244.86 70.22 51.74 Pentamethylbenzene c -128.13 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 25.64 70.22 51.74 Pentanal g -54.45 -25.88 91.53 29.96 Pentanamide c -90.70 95.1 28.7 Pentan-2,4-dione liq -101.33 29.96 quactylacetone) g -90.47 95.1 28.7 Pentanel g -35.00 -2.00 83.40 28.73 1-Pentanel liq -35.72 2.28 74.18 74.18 Pentanociacid liq -35.72 2.28 74.18	Pentafluorobenzoic acid	c	-296.34			
Pentamethylbenzene liq -32.33 25.64 70.22 51.74 Pentamethylbenzoic acid c -128.13 -25.88 91.53 29.96 Pentanalide c -90.70 -90.70 95.1 28.7 Pentan-2,4-dione liq -101.33 99.9 95.1 28.7 Pentan-1,5-dithiol liq -30.99 9.0.47 95.1 28.7 Pentan-1,5-dithiol liq -35.72 2.28 74.18 28.73 Pentanolic acid liq -35.72 2.28 74.18 28.73 Pentanolic acid liq -35.72 2.28 74.18 74.18 Pentanolic acid liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 -38.3 62.0 49.8 3-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanol g -61.82 -32.76 89.91 28.91 3-Pentanone liq		g		-246.00	79.76	22.88
Pentamethylbenzoic acid 1-Pentanal c -128.13 -25.88 91.53 29.96 Pentanamide c -90.70 Pentan-24-dione liq -101.33 29.96 Pentan-2,4-dione liq -101.33 95.1 28.7 Pentane g -90.47 95.1 28.7 Pentane g -90.47 95.1 28.7 Pentanel liq -30.99 75.00 83.40 28.73 Pentanel liq -35.72 2.28 74.18 74.18 Pentanociacid liq -35.72 2.28 74.18 74.18 Pentanociacid liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 3.3 62.0 49.8 2-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 17.17 82.65 26.	Pentafluorophenol	С	-244.86			
1-Pentananide		liq		25.64	70.22	51.74
Pentanamide c -90.70 Pentan-2,4-dione liq -101.33 (acetylacetone) g -90.47 95.1 28.7 Pentan-1,5-dithiol liq -30.99 -2.00 83.40 28.73 Pentane g -35.00 -2.00 83.40 28.73 1-Pentanethiol liq -35.72 2.28 74.18 Pentanoic acid liq -133.71 -89.10 62.10 50.48 (valeric acid) liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 38.3 62.0 49.8 2-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone liq -70.87 89.91 28.91 3-Pentanone liq -70.87 18.91 82.65 26.19 2-Pentene g -5.00 18.91 82.65 26.19 2-Pentene g -7.59 16.71 81.36 25.92	*	С				
Pentan-2,4-dione (acetylacetone) liq g = -90.47 95.1 28.7 Pentan-1,5-dithiol liq = -30.99 9 28.7 28.7 Pentane pentane g = -35.00 -2.00 83.40 28.73 1-Pentanethiol liq = -35.72 2.28 74.18 Pentanoic acid (valeric acid) liq = -133.71 -89.10 62.10 50.48 L-Pentanoid liq = -85.0 -38.3 62.0 49.8 2-Pentanol liq = -87.7 -89.10 62.10 50.48 2-Pentanol liq = -87.7 -89.10 62.0 49.8 2-Pentanol liq = -87.7 -89.10 62.0 49.8 2-Pentanol liq = -87.7 -89.10 62.0 49.8 2-Pentanol liq = -88.5 -40.4 57.4 60.0 29.8 2-Pentanone liq = -61.82 -32.76 89.91 28.91 28.91 3-Pentanone liq = -70.87 17.17 82.65 26.19 29.91 29.91 29.91 29.91 29.91 <td></td> <td>g</td> <td></td> <td>-25.88</td> <td>91.53</td> <td>29.96</td>		g		-25.88	91.53	29.96
(acetylacetone) g -90.47 95.1 28.7 Pentane 1,5-dithiol liq -30.99 28.73 28.73 Pentane 2 g -35.00 -2.00 83.40 28.73 1-Pentanethiol liq -35.72 2.28 74.18 Pentanoic acid liq -133.71 -89.10 62.10 50.48 (valeric acid) liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 3.3 62.0 49.8 2-Pentanol liq -87.7 3.276 89.91 28.91 3-Pentanone liq -70.87 18.91 82.65 26.19 2-Pentenne g -6.71 17.17 82.76 24.32 2-Pentenne g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7 16.71 81.36 25.92 2-Pentyne g 34.50 50.25 78.82 25.50						
Pentan-1,5-dithiol liq -30.99 -2.00 83.40 28.73 1-Pentanethiol liq -35.72 2.28 74.18 Pentanoic acid (valeric acid) liq -133.71 -89.10 62.10 50.48 1-Pentanol liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 3.8 62.0 49.8 2-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 18.91 82.65 26.19 2-Pentene g -5.00 18.91 82.65 26.19 2-Pentene g -6.71 17.17 82.76 24.32 2-Pentene g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7 3-9.40 46.41 79.30 23.59 2-Pentyne g 34.50 50.2	· · · · · · · · · · · · · · · · · · ·	liq				
Pentane g -35.00 -2.00 83.40 28.73 1-Pentanethiol liq -35.72 2.28 74.18 50.48 Pentanoic acid liq -133.71 -89.10 62.10 50.48 (valeric acid) liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 3.83 62.0 49.8 2-Pentanol liq -87.7 3.83 62.0 49.8 2-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 1 1.71.7 82.65 26.19 2-Pentanone g -5.00 18.91 82.65 26.19 2-Pentanone g -6.71 17.17 82.65 26.19 2-Pentene g -6.71 17.17 82.65 26.19 2-Pentene acis g -6.71					95.1	28.7
1-Pentanethiol	· · · · · · · · · · · · · · · · · · ·	liq				
Pentanoic acid (valeric acid) liq (valeric acid) -133.71 -89.10 62.10 50.48 1-Pentanol liq -88.5 -38.3 62.0 49.8 2-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 -70.87 18.91 82.65 26.19 2-Pentene g -7.59 17.17 82.76 24.32 24.32 25.92 2-Pentenoic acid liq -106.7 16.71 81.36 25.92 25.92 2-Pentenoic acid liq -106.7 16.71 81.36 25.92 25.50 29.2						28.73
(valeric acid) liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 3-Pentanol liq -87.7 3-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 18.91 82.65 26.19 2-Pentanone g -5.00 18.91 82.65 26.19 2-Pentanone g -6.71 17.17 82.76 24.32 2-Pentene g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7 31.36 25.92 25.92 3-Pentenoic acid liq -102.9 1-10.29 46.41 79.30 23.59 3-Pentyne g 30.80 46.41 79.30 23.59 Perylene c 43.69 44.22.67 94.02 70.93 Phenacetin c -101.1						
1-Pentanol liq -85.0 -38.3 62.0 49.8 2-Pentanol liq -87.7 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 -70.93<		liq	-133.71	-89.10	62.10	50.48
2-Pentanol liq -87.7 3-Pentanol liq -88.5 -40.4 57.4 60.0 2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 18.91 82.65 26.19 2-Pentene g -5.00 18.91 82.65 26.19 2-Pentene g -6.71 17.17 82.76 24.32 2-Pentene g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7 16.71 81.36 25.92 2-Pentenoic acid liq -103.9 4.641 79.30 23.59 2-Pentyne g 34.50 50.25 78.82 25.50 2-Pentyne g 30.80 46.41 79.30 23.59 Perylene c 43.69 -422.67 94.02 70.93 Perylene c 27.3 64.12 50.6 Phenactin c		4.				40.0
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				-38.3	62.0	49.8
2-Pentanone g -61.82 -32.76 89.91 28.91 3-Pentanone liq -70.87 -70.92 -70.92 -70.93 </td <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						
1-Pentene g -5.00 18.91 82.65 26.19 2-Pentene g -6.71 17.17 82.76 24.32 $trans$ g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7		_		-32.76	89.91	28.91
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		g	-5.00	18.91	82.65	26.19
trans g -7.59 16.71 81.36 25.92 2-Pentenoic acid liq -106.7 -103.9 -102.9			6.71	15.15	02.76	24.22
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						
3-Pentenoic acid				16.71	81.36	25.92
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		_				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-		50.25	70.02	25.50
Perfluoropiperidine liq -482.9 -422.67 94.02 70.93 Perylene c 43.69 -14.3	•					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		_				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		_		-422.67	94.02	70.93
Phenacetin c -101.1 50.6 9,10-Phenanthraquinone c -55.18 50.6 Phenanthrene c 27.3 64.12 50.6 Phenazine c 56.4 -12.05 34.42 32.2 Phenol g -23.03 -7.86 75.43 24.75 Phenoxy radical g 10 75.43 24.75 Phenoxyacetic acid c -122.8 71 75.43 24.75						
9,10-Phenanthraquinone c -55.18 50.6 Phenanthrene c 27.3 64.12 50.6 Phenazine c 56.4 -12.05 34.42 32.2 Phenol c -37.80 -11.02 30.46 g -23.03 -7.86 75.43 24.75 Phenoxy radical g 10 Phenoxyacetic acid c -122.8 Phenyl radical g 71						
Phenanthrene c 27.3 64.12 50.6 Phenazine c 56.4 -12.05 34.42 32.2 Phenol c -37.80 -11.02 30.46 g -23.03 -7.86 75.43 24.75 Phenoxy radical g 10 75.43 24.75 Phenoxyacetic acid c -122.8 71 75.43 24.75						
Phenazine c 56.4 Phenol c -39.44 -12.05 34.42 32.2 liq -37.80 -11.02 30.46 g -23.03 -7.86 75.43 24.75 Phenoxy radical g 10 Phenoxyacetic acid c -122.8 Phenyl radical g 71	•			64.12	50.6	
Phenol c -39.44 -12.05 34.42 32.2 liq -37.80 -11.02 30.46 g -23.03 -7.86 75.43 24.75 Phenoxy radical g 10 75.43 24.75 Phenoxy acetic acid c -122.8 71 75.43 75.43				04.12	30.6	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				_12.05	34.42	32.2
g	I HEHOI				34.42	
Phenoxy radical g 10 Phenoxyacetic acid c -122.8 Phenyl radical g 71					75.42	
Phenoxyacetic acid c -122.8 Phenyl radical g 71	Dhanovy radical	_		- 7.80	13.43	24.73
Phenyl radical g 71	*	_				
	•					
I nerry i accetate nq 00.02	•					
		114	00.02			

5.34 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

		$\Delta H f^{\circ}$,	$\Delta G f^{\circ}$,	S° , cal $\cdot \deg^{-1} \cdot$	C_p° , cal $\cdot \deg^{-1} \cdot$
Substance	State	kcal⋅mol ⁻¹	kcal·mol ⁻¹	mol ⁻¹	mol ⁻¹
Phenylacetic acid	С	-95.3			
Phenylacetylene	g	78.22	86.46	76.88	27.46
β-Phenyl-1-alanine, DL- and L-	c	-111.9	-50.6	51.06	48.52
Phenyl benzoate	С	-57.7			
2-Phenylbenzoic acid	c	-83.4			
Phenylboronic acid	c	-172.0			
1-Phenylcyclohexene	liq	-4.0			
Phenylcyclopropane	liq	24.7			
<i>N</i> -Phenyldiacetimide	c	-86.63			
<i>p</i> -Phenylenediamine	c	0.73			
Phenyl ethyl sulfide	liq	5.29			
DL-Phenylglyceric acid	c	-178.5			
<i>N</i> -Phenylglycine	С	-96.2			
<i>a</i> -Phenylglycine	С	-103.2			
Phenylglyoxime					
α	c	-4.9			
β	c	10.1			
Phenylglyoxylic acid	c	-115.3			
Phenylhydrazine	liq	34.03			
Phenyl methyl sulfide	liq	11.5			
N-Phenyl-2-naphthylamine	c	38.2			
N-Phenylpyrrole	С	38.1			
2-Phenylpyrrole	c	34.5			
Phenyl salicylate	С	-104.3			
Phenyl thiolacetate	liq	-29.16			
Phosgene	g	-52.80	-49.42	67.82	13.79
Phthalamide	С	-104.4			
<i>m</i> -Phthalic acid	С	-191.91			
o-Phthalic acid	С	-186.91	-141.39	49.7	45.0
<i>p</i> -Phthalic acid	С	-195.05			
Phthalic anhydride	С	-110.1	-79.12	42.9	38.5
Phthalonitrile	С	65.82			
Pimelic acid	С	-241.25			
(heptanedioic acid)					
Pinene		2.0			
α	liq	-3.9			
β	liq	-1.8			
Piperazine	C 1:-	-10.90			
Piperidine	liq	-21.05	26.70	20.4	
α-Piperidone	c	-73.3	-26.79	39.4	
DL-Proline	С	-125.7	49.27	59.20	14.10
Propadiene	g	45.92	48.37	58.30	14.10
Propane	g	-24.82	-5.63	64.58	17.59
1,2-Propanediamine	liq	-23.38			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	C_p° , $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot \operatorname{mol}^{-1}$
1,2-Propanediol	liq	-119.6			
1,3-Propanediol	liq	-124.4			
1,3-Propanedithiol	liq	-18.83			
2,3-Propanedithiol	liq	-18.82			
1-Propanethiol		-16.22	0.52	80.40	22.65
2-Propanethiol	g	-18.22 -18.22	-0.61	77.51	
	g				22.94
1-Propanol	liq	-72.66	-40.78	46.5	33.7
2.5	g	-61.28	-38.67	77.61	20.82
2-Propanol	liq	-75.97	-43.09	43.16	36.06
	g	-65.11	-41.44	74.07	21.21
1,2,3-Propenetricarboxylic					
acid					
cis	С	-292.7			
trans	c	-294.7			
2-Propen-1-ol	g	-31.55	-17.03	73.51	18.17
(allyl alcohol)					
Propionaldehyde	g	-45.90	-31.18	72.83	18.80
Propionamide	c	-81.7			
Propionic acid	liq	-122.07	-91.65		
Propionic anhydride	liq	-161.53	-113.66		
Propionitrile	liq	3.5	21.31	45.25	
•	g	12.10	22.98	68.50	17.46
1-Propylamine	g	-17.30	9.51	77.48	22.89
2-Propylamine	liq	-26.83			
Propylbenzene	g	1.87	32.80	95.76	36.41
Propylcarbamate	c	-132.07			
Propyl chloroacetate	liq	-123.3			
Propylcyclohexane	g	-46.20	11.31	100.27	44.03
Propylcyclopentane	g	-35.39	12.57	99.73	36.96
Propylene (propene)	g	4.88	15.02	63.72	15.37
Propylene oxide	g	-22.17	-6.16	68.53	17.29
Propyl nitrate	g	-41.60	-6.53	92.10	28.99
Propyl phenyl ketone	liq	-45.14	0.55	72.10	20.77
Propyl thiolacetate	liq	-70.29			
Propyl trichloroacetate	liq	-122.7			
Propyne (methyl		44.32	46.47	59.30	14.50
acetylene)	g	77.32	10.77	37.30	14.50
•		22 /1			
Pyrazine	С	33.41			
Pyrazole	С	28.3	64.40	52.75	56.1
Pyrene	C	27.44	64.40	53.75	56.4
Pyridazine	liq	53.74	42.24	12.52	21.72
Pyridine	liq	23.96	43.34	42.52	31.72
D ' '!'	g	33.61	45.46	67.59	18.67
Pyrimidine	liq	35.04			
Pyrrole	liq	15.08	I	I .	I .

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

			1	I	
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Pyrrole-2-aldehyde	c	-24.8			
Pyrrole-2-aldoxime	c	2.9			
Pyrrolidine	liq	-9.84	25.94	48.76	
1 yrrondine	*	-0.86	27.41	73.97	19.39
2 P1: d	g		27.41	13.91	19.39
2-Pyrrolidone	c	-68.3	110.75	42.0	
Pyruvic acid	liq	-139.7	-110.75	42.9	
Quinaldine	c	39.3			
Quinhydrone	c	-19.79	-77.19	77.9	66.2
Quinidine	c	-38.3			
Quinine	c	-37.1			
Quinoline	liq	37.33	65.90	51.9	
p-Quinone	c 1	-44.10	-20.0	38.9	
Raffinose	c	-761			
L-Rhamnose	c	-761 -256.5			
Rhamnose triacetate	c	-250.5 -455.4			
	_				
D-Ribose	С	-251.16			
Saccharinic acid lactone	c	-249.6			
Salicylaldehyde	liq	-66.9			
Salicylaldoxime	c	-43.91			
Salicyclic acid	c	-140.9	-99.93	42.6	
Sarcosine	c	-121.2			
Sebacic acid	c	-258.8			
(decanedioic acid)					
Semicarbazide, std state,	aq	-39.9	-9.7	71.2	
m = 1	1				
L-Serine	c	-173.6			
Serylserine	c	-281.8			
Sorbic acid	С	-93.4			
L-Sorbose	С	-303.68	-217.10	52.8	
5,5'-Spirobis(1,3-dioxane)	c	-167.8			
Spiropentane	g	44.27	63.41	67.45	21.06
Stearic acid	c	-226.5		31110	
(octadecanoic acid)					
Stilbene					
cis	liq	43.81			
trans	c	32.27	75.90	60.0	
Strychnine	c	-41.0	,,,,,	00.0	
Styrene	liq	24.83	48.37	56.78	43.64
55,10110	g	35.22	51.10	82.48	29.18
Suberic acid	c g	-248.1	31.10	02.40	27.10
(octanedioic acid)		2-70.1			
Succinamide	c	-138.9			
Succinic acid	c	-224.79	-178.64	42.0	35.8
Sucrose	c	2531.9	2369.18	86.1	33.0
		2551.7	2307.10	00.1	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
L-Tartaric acid	С	-306.5			
DL-Tartaric acid	c	-308.5			
meso-Tartaric acid	c	-305.9			
Tetrabromomethane		19.00	15.61	85.53	21.78
	g		13.01	65.55	21.70
Tetracene	С	37.95			
Tetrachlorobenzoquinone	С	-69.0	07.2	01.5	20.5
1,1,1,2-Tetrachlorodi-	g	-117.1	-97.3	91.5	29.5
fluoroethane		25.5	10.0	05.05	24.65
1,1,1,2-Tetrachloroethane	g	-35.7	-19.2	85.05	24.67
1,1,2,2-Tetrachloroethane	liq	-47.0	-22.7	59.0	39.6
	g	-36.50	-20.45	86.69	24.09
Tetrachloroethylene	g	-3.40	4.90	81.46	22.69
Tetrachloromethane	liq	-31.75	-14.97	51.67	
	g	-22.90	-12.80	74.07	19.94
1,1,2,2-Tetracyano- cyclopropane	С	141			
Tetracyanoethylene	С	149.1			
Tetradecane	g	-79.38	15.97	167.40	77.93
Tetradecanoic acid	c	-199.2			
1-Tetradecene	g	-49.36	36.99	166.40	75.36
Tetraethylene glycol	liq	-234.6			
Tetraethyllead	liq	12.7	80.4	112.92	
•	g	26.3			
1,1,1,2-Tetrafluoroethane	g	-214.10	-197.46	75.58	20.62
Tetrafluoroethylene	g	-157.40	-149.07	71.69	19.24
Tetrafluoromethane	g	-223.0	-212.3	62.45	14.59
Tetrahydrofuran	liq	-51.67	212.0	02.10	11.05
Tetrahydrofurfuryl alcohol	liq	-104.1			
1,2,3,4-Tetrahydro-	liq	-6.1			
naphthalene (Tetralin)	nq	0.1			
Tetrahydropyran	liq	-61.1			
1,2,5,6-Tetrahydropyridine	liq	8.0			
Tetraiodomethane	g	62.84	51.89	93.60	22.91
1,2,3,4-Tetramethylbenzene	liq	-23.0	25.49	69.45	22.71
1,2,3,5-Tetramethylbenzene	liq	-23.54	23.58	99.55	57.5
1,2,4,5-Tetramethylbenzene	liq	-29.48	24.20	71.83	51.6
2,2,3,3-Tetramethylbutane		-53.99	5.26	93.06	31.0
Tetramethyllead	g	23.5	62.8	76.5	
renamentyneau	liq	32.6	64.7	100.5	34.42
Totromothylailana	g				
Tetramethylsilane	g	-68.50	-23.92	86.30	31.12
Tetramethylsuccinic acid	c	-242.0			
Tetramethylthia-	С	-19.84			
cyclopropane	1.				
Tetranitromethane	liq	8.9			
1,1,1,2-Tetraphenylethane	С	53.31			
	l			l	L

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol $^{-1}$	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal $\cdot \deg^{-1} \cdot \operatorname{mol}^{-1}$
1,1,2,2-Tetraphenylethane	с	51.63			
Tetraphenylethene	c	74.46			
Tetraphenylhydrazine	c	109.4			
Tetraphenylmethane	c	59.1	137.20		
Tetrazole	c	56.7			
Thebaine	c	-63.0			
Theobromine	c	-86.4			
Thiaadamantane	c	-34.22			
2-Thiabutane	liq	-21.89	1.79	57.14	
	g	-14.25	2.73	79.62	22.73
Thiacyclobutane	g	14.61	25.69	68.17	16.57
Thiacycloheptane	g	-14.66	20.09	86.50	29.78
Thiacyclohexane	liq	-25.32	9.96	52.16	
•	g	-15.12	12.68	77.26	25.86
Thiacyclopentane	liq	-17.39	8.97	49.67	
• •	g	-8.08	11.00	73.94	21.72
Thiacyclopropane	liq	12.41	22.52	38.84	
	g	19.65	23.16	61.01	12.83
4-Thia-5,5-dimethylhex-	liq	-21.68			
1-ene					
2-Thiaheptane	g	-29.34	8.39	107.73	39.10
3-Thiaheptane	g	-29.92	7.65	108.27	38.71
4-Thiaheptane	liq	-40.62	5.12	80.85	
	g	-29.96	7.94	107.16	38.53
2-Thiahexane	liq	-34.15	4.08	73.49	
	g	-24.42	6.37	98.43	33.64
3-Thiahexane	liq	-34.58	3.50	73.98	
	g	-25.00	5.63	98.97	33.25
5-Thianonane	liq	-52.74	7.66	96.82	
	g	-39.99	11.76	125.76	49.46
2-Thiapentane	liq	-28.21	2.79	65.14	
	g	-19.54	4.40	88.84	28.05
3-Thiapentane	liq	-28.43	2.81	64.36	40.97
	g	-19.95	4.25	87.96	27.97
2-Thiapropane	g	-8.97	1.66	68.32	17.71
6-Thiaundecane	liq	-63.61			
Thioacetic acid	g	-43.49	-36.81	74.86	19.33
Thiohydantoic acid	c	-132.6			
Thiohydantoin	c	-59.5			
Thiolacetic acid	liq	-52.39			
β-Thiolactic acid	liq	-111.6			
Thiophene	liq	19.24	28.97	43.30	
*	g	27.66	30.30	66.65	17.42
Thiosemicarbazide	c	6.0			
	1		I		1
Thiourea	c	-21.13	5.2	27.7	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	C_p° , cal · deg ⁻¹ mol ⁻¹
Threonine, L- and DL-	С	-181.4			
Thymine	c	-111.9			
Thymol	c	-74.0			
Tiglic acid	С	-117.3			
Toluene	liq	2.87	27.19	52.81	37.58
	g	11.95	29.16	76.64	24.77
2-Toluenethiol	liq	10.57			
m-Toluic acid	c	-101.85			
o-Toluic acid	С	-99.55			
p-Toluic acid	c	-102.59			
o-Toluic anhydride	С	-127.5			
<i>p</i> -Toluic anhyride	c	-124.5			
Trehalose	c	-531.3			
2.4.6-Triamino-	c	-17.3	44.10	35.63	
1,3,5-triazine	g	-17.13	42.33	74.10	20.93
(triaminotriazine)	8				
2-Triazoethanol	liq	22.6			
Tribenzylamine	c	33.6			
Tribromochloromethane	g	3.0	2.17	85.36	
Tribromofluoromethane	g	-45.4	-46.14	82.65	
Tribromomethane	g	4.00	1.78	79.01	16.96
Tributylamine	liq	-67.32	11.70	,,,,,,	10.70
Tributyl borate	liq	-286.7			
Tributylboron	liq	-83.4			
Tributyl phosphate	liq	-348			
Tributylphosphine oxide	c	-110			
Trichloroacetaldehyde	liq	-56.1			
Trichloroacetamide	c	-85.6			
Trichloroacetic acid	c	-120.7			
Ionized	aq	-123.4			
Trichloroacetyl chloride	lig	-66.4			
Trichlorobenzoquinone	c	-64.5			
1,1,1-Trichloroethane	g	-34.01	-18.21	76.49	22.07
1,1,2-Trichloroethane	g	-33.10	-18.52	80.57	21.47
Trichloroethylene	g	-1.40	4.75	77.63	19.17
Trichlorofluoromethane	g	-68.10	-58.68	74.06	18.66
Trichloromethyl	g	19	22	70.9	15.21
1,2,3-Trichloropropane	g	-44.40	-23.37	91.52	26.82
1,1,1-Tricyanoethane	c	83.9			
Tricyanoethylene	c	105.0			
Tridecane	g	-74.45	13.97	158.09	72.47
Tridecanoic acid	c	-192.8			
1-Tridecene	g	-44.45	34.96	157.09	69.89
Triethylaluminum	liq	-56.6			

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TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

	I		ı	ı	
Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Triethylamine	g	-23.80	26.36	96.90	38.46
Triethylaminoborane	liq	-47.47			
Triethyl arsenite	liq	-168.9			
Triethylarsine	liq	3.1			
Triethyl borate	liq	-250.4			
Triethylenediamine	c c	-3.4	57.28	37.67	
Triethylene glycol	liq	-192.2			
Triethyl phosphate	liq	-297			
Triethylphosphine	liq	-21.3			
Triethyl phosphite	liq	-205.9			
Triethylstibine	liq	1.2			
Triethylsuccinic acid	c	-254.9			
Triethyl thionophosphate	liq	-232.5			
Trifluoroacetic acid	liq	-255.4			
Trifluoroacetonitrile	g	-118.4	-110.4	71.3	18.70
1,1,1-Trifluoroethane	g	-178.20	-162.11	68.67	18.76
2,2,2-Trifluoroethanol	liq	-207.4			
Trifluoroethylene	g	-118.50	-112.22	69.94	16.54
Trifluoroiodomethane	g	-141.0	-136.70	73.50	
Trifluoromethane	g	-165.71	-157.48	62.04	12.22
Trifluoromethyl					
CF₃•	g	-112.4	-109.2	63.3	11.90
CF_3^+	g	100.6	103.1	60.8	11.87
Trifluoromethylbenzene	liq	-152.40	-123.98	64.89	
	g	-143.42	-122.20	89.05	31.17
Trifluoromethylhypo- fluorite (CF ₃ OF)	g	-183	-169	77.06	18.97
DL-Trihydroxyglutaric acid	С	-356			
Triiodomethane	g	50.40	42.54	84.97	17.94
Trimethylacetic acid	liq	-134.9			
Trimethylacetic anhydride	liq	-186.4			
2,4,5-Trimethylaceto- phenone	liq	-60.3			
2,4,6-Trimethylaceto- phenone	liq	-63.9			
Trimethylaluminum	liq	-36.1		50.05	37.19
Trimethylamine	g	-5.70	23.64	69.02	21.93
Std state, molarity = 1	aq	-18.17	22.22	31.9	
Trimethylamine aluminum chloride adduct	c	-210.1		2-13	
Trimethylammonium ion Std state, molarity = 1	aq	-26.99	8.90	47.0	
Trimethyl arsenite	liq	-141.2			
Trimethylarsine Trimethylarsine	liq	-3.9			
11111ctily lai silic	114	3.7			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal $\cdot \deg^{-1} \cdot \mod^{-1}$	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,2.3-Trimethylbenzene	liq	-14.01	25.68	66.40	
1,2,4-Trimethylbenzene	liq	-14.79	24.46	67.93	
1,3,5-Trimethylbenzene	liq	-15.18	24.83	65.38	
Trimethyl borate	liq	-222.9			
Trimethylboron	liq	-34.1			
2,2,3-Trimethylbutane	g	-48.95	1.02	91.61	39.33
Trimethylchlorosilane	liq	-91.8			
cis,cis-1,3,5-Trimethyl- cyclohexane	g	-51.48	8.10	93.30	42.93
2,2,3-Trimethylpentane	liq	-61.44	2.21	78.30	
, , , , , , , , , , , , , , , , , , ,	g	-52.61	4.09	101.62	
2,2,4-Trimethylpentane	liq	-61.97	1.65	78.40	
• •	g	-53.57	3.27	101.15	
2,3,3-Trimethylpentane	liq	-60.63	2.54	79.93	
• •	g	-51.73	4.52	103.14	
2,3,4-Trimethylpentane	liq	-60.98	2.55	78.71	
	g	-51.97	4.52	102.31	
2,4,4-Trimethyl-1-pentene	liq	-35.21	20.66	73.2	
2,4,4-Trimethyl-2-pentene	liq	-34.44	21.04	74.5	
Trimethylphosphine	liq	-29.2			
Trimethylphosphine- N-ethylimine	liq	-35.8			
Trimethylphosphine oxide	c	-114.2			
Trimethyl phosphite	liq	-177.1			
Trimethylsilanol	liq	-130.3			
Trimethylstibine	liq	0.2			
Trimethylsuccinic acid	c	-239.2			
Trimethylsuccinic anhydride	С	-164.5			
Trimethylthiacyclopropane	liq	-14.47			
Trimethylurea	c	-79.0			
2,4,6-Trinitroanisole	c	-37.6			
1,3,5-Trinitrobenzene	c	-10.40			
Trinitromethane	c	-11.50			
1,4,5-Trinitronaphthalene	c	8.7			
1,3,8-Trinitronaphthalene	c	5.8			
2,4,6-Trinitrophenetole	c	-48.9			
2,4,6-Trinitrophenol	c	-51.23			
2,4,6-Trinitrophenyl- hydrazine	С	8.8			
2,4,6-Trinitrotoluene	c	-16.0			
2,4,6-Trinitro- <i>m</i> -xylene	c	-24.5			
Triphenylamine	c	58.70 ^{18°C}	120.50		
Triphenylarsine	c	74.1			
Triphenylcarbinol	С	-0.80	65.2	78.7	

5.42 SECTION 5

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , $cal \cdot deg^{-1} \cdot mol^{-1}$	$C_p^{\circ},$ $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot$ mol^{-1}
Triphenylene	c	33.72	78.68	60.87	
1,1,1-Triphenylethane	c	37.56	, 0.00	00.07	
1,1,2-Triphenylethane	c	31.11			
Triphenylethylene	c	55.8	123.00		
Triphenylmethane	c	38.71	98.60	74.6	70.5
Triphenyl phosphate	c	-181	70.00	7 1.0	70.5
Triphenylphosphine	c	55.5			
Triphenylphosphine oxide	c	-14.4			
Tripropylamine Tripropylamine	liq	-49.51			
Tris(acetylacetonato)- chromium	c	-366.4			
1,1,1-Tris(hydroxymethyl)- ethane	c	-177.96			
Tropolone	c	-57.18			
L-Tryptophan	c	-99.8	-28.54	60.00	56.92
L-Tyrosine	С	-163.4	-92.18	51.15	51.73
Undecane	liq	-78.05	5.44	109.49	
	g	-64.60	9.94	139.48	61.53
1-Undecene	g	-34.60	30.94	138.48	58.96
Urea	c	-79.71	-47.19	25.00	22.26
Std state, $m = 1$	aq	-75.95	.,,,,		
Urea nitrate	c	-134.8			
Urea oxalate	c	-365.3			
Uric acid	c	-147.73	-85.75	41.4	
Valeric acid	liq	-133.71	-89.10	62.10	50.48
Valine, L and DL-	c	-133.71 -148.2	-85.80	42.75	40.35
Valylphenylalanine	c	-183.5	65.60	42.73	40.55
Veronal	c	-178.7			
Vinyl radical	g	63			
Vinyl bromide	g	18.7	19.3	65.90	13.27
Vinyl chloride	g	8.5	12.4	63.07	12.84
Vinylcyclohexane	liq	-21.19	12.4	03.07	12.04
Vinyleyclopropane	liq	29.3			
2-Vinylpyridine	liq	37.2			
5 15	1 1		20.64	20.5	
Xanthine	c	-90.49	-39.64	38.5	44.0
o-Xylene	liq	-5.84	26.37	58.91	44.9
V-1	g 1: -	4.54	29.18	84.31	31.85
<i>m</i> -Xylene	liq	-6.08	25.73	60.27	43.8
V1	g 1: -	4.12	28.41	85.49	30.49
<i>p</i> -Xylene	liq	-5.84	26.31	59.12	20.22
0.2 V-11	g	4.29	28.95	84.23	30.32
2,3-Xylenol	g	-37.57			
2,4-Xylenol	g	-38.93 -38.63			
2,5-Xylenol	g	-38.63			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	$\Delta H f^{\circ}$, kcal·mol ⁻¹	$\Delta G f^{\circ}$, kcal·mol ⁻¹	S° , cal \cdot deg ⁻¹ \cdot mol ⁻¹	C_p° , $\operatorname{cal} \cdot \operatorname{deg}^{-1} \cdot \operatorname{mol}^{-1}$
2,6-Xylenol 3,4-Xylenol 3,5-Xylenol Xylitol D-Xylose	g g g c c	-38.66 -37.42 -38.61 -267.32 -252.8			

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds

Abbreviations Used in the Table

 ΔHm , enthalpy of melting (at the melting point) in kcal·mol⁻¹

 ΔHv , enthalpy of vaporization (at the boiling point) in kcal·mol⁻¹

 ΔHs , enthalpy of sublimation (at 298 K) in kcal·mol⁻¹

 C_p , specific heat (at temperature specified, measured on the Kelvin scale) for physical state in existence at that temperature, expressed in cal \cdot K⁻¹·mol⁻¹

 ΔHt , enthalpy of transition (at temperature specified, measured in degrees Celsius) in kcal·mol⁻¹

					C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Acenaphthene			20.6					
Acenaphthylene			17.0					
Acetaldehyde	0.770	6.24		15.73	20.52	24.20	29.96	
Acetanilide			19.3					
Acetic acid	2.80	5.663		19.52	25.15	29.08	31.99	
Acetic anhydride	2.51	9.85	11.54	30.86	41.62	48.91	54.11	
Acetone	1.366	6.952		22.00	29.34	34.93	39.15	
Acetonitrile $(\Delta Ht, 0.215 \text{ at } -56 ^{\circ}\text{C})$	1.952	7.3	7.94	14.62	18.35	21.26	23.50	
Acetophenone		9.275	13.4					
Acetyl bromide			7.9					
Acetyl chloride			7.2	18.86	23.18	26.30	28.60	
Acetylene	0.900	4.05	5.1	11.97	13.73	14.93	15.92	
Acetylenedicarbonitrile			6.88	22.66	25.37	27.26	28.62	
Acetyl fluoride			6.0					
Acetyl iodide			7.9					
Acrylic acid		11.21	12.98	22.94	29.50	33.93	37.12	
Acrylonitrile		7.8		18.36	23.11	26.43	28.88	
Adenine			25.8					

Adipic acid α-Alanine Allyl ethyl sulfoxide Allyl trichloroacetate 1-Aminobutane 2-Aminobutane Aniline Anthracene 9,10-Anthracenedione Azoisopropane Azulene	2.519	10.643 13.5	30.8 33.0 17.1 12.5 8.50 7.5 13.325 24.7 26.8 8.5 22.8	35.44 35.40 34.17	47.30 47.55 46.09	56.01 56.42 53.79	62.54 62.54 69.18
Benzaldehyde			12				
1,2-Benzanthra-9,10-quinone			19.8				
Benzene	2.358	7.352	8.090	26.74	37.73	45.06	50.16
Benzenethiol	2.736	9.53	11.64	32.76	44.13	51.59	56.79
Benzil Benzoic acid	4.32	12.10	23.5 22.70				
Benzoic acid Benzoic anhydride	4.52	12.10	23.70				
Benzonitrile	2.60	11.0	13.26	33.65	44.80	52.08	57.08
Benzophenone	2.00	11.0	22.5	33.03	44.00	32.08	37.08
1,4-Benzoquinone			15.00				
Benzoyl bromide			14.0				
Benzoyl chloride			13.1				
Benzoyl iodide			14.8				
3,4-Benzophenanthrene			25.4				
Benzyl bromide			11.3				
Benzyl chloride			12.3				
Benzyl ethyl sulfide			13.6				
Benzyl iodide			11.3				
Benzyl methyl ketone			12.78				
Benzyl methyl sulfide			12.8				
Bicyclo[4.1.0]heptane			9.14				
Bicyclo[3.1.0]hexane			7.85				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

					C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Bicyclo[4.2.0]octane			9.85					
Bicyclo[5.1.0]octane			10.42					
Bicyclopropyl			8.0					
Biphenyl	4.44	10.9		52.83	73.54	86.92	96.00	
Biphenylene			30.8					
Bromobenzene	2.54	9.05	10.62	30.44	40.99	47.78	52.40	
4-Bromobenzoic acid			21.0					
1-Bromobutane	1.6	7.78		32.64	43.00	50.48	56.03	
2-Bromobutane			8.45	33.09	43.76	51.31	56.93	
Bromoethane	1.4	6.41	6.57	18.93	24.56	28.58	31.59	
Bromoethene				15.91	19.83	22.50	24.46	
1-Bromoheptane			12.05					
1-Bromohexane			10.91					
Bromomethane ΔHt , 0.113 at -99.4 °C	1.429	5.715		11.94	14.98	17.26	19.01	
2-Bromo-2-methylpropane ΔHt , 1.35 at -64.5 °C; 0.25 at -41.6 °C	0.47		7.4	34.93	45.58	52.65	57.74	
1-Bromooctane			13.14					
1-Bromopentane	2.74	8.24		39.58	52.34	61.55	68.36	
1-Bromopropane	1.56	7.14		25.70	33.66	39.41	43.70	
2-Bromopropane		6.79		26.34	34.42	40.09	44.26	
1,2-Butadiene	1.665	5.82	5.71	23.54	30.72	36.01	40.02	
1,3-Butadiene	1.908	5.42	5.03	24.29	31.84	36.84	40.52	
<i>n</i> -Butadiene sulfone			14.7					
Butadiyne				20.17	23.14	25.11	26.61	
Butane ΔHt , 0.494 at -165.60 °C	1.114	5.352	5.035	29.60	40.30	48.23	54.22	
2,3-Butanedione			9.25					
1,4-Butanedithiol			13.22					
1-Butanethiol	2.500	7.702	8.73	34.95	46.54	55.68	62.95	

2-Butanethiol	1.548	7.312	8.14	35.38	46.42	54.29	60.02
1-Butanol	2.24	10.31	12.52	32.80	43.90	52.11	58.26
2-Butanol		9.75	11.87	33.70	44.72	52.68	58.62
2-Butanone	2.017	7.475	8.34	29.81	39.09	46.08	51.33
1-Butene	0.920	5.238	4.81	26.04	35.14	41.80	46.82
2-Butene							
cis	1.747		5.29	24.33	33.80	40.87	46.15
trans	2.332	5.580	5.10	26.02	34.80	44.20	46.58
1-Buten-3-yne		5.439		21.26	26.67	30.40	33.16
N-Butylacetamide			18.2				
Butyl acetate			10.42				
tert-Butylamine		8.58	7.10	36.46	48.87	57.49	63.79
Butylbenzene							
stable(I)	2.682(I)		11.98	54.75	75.20	89.37	99.49
metastable(II)	2.691(11)	9.38					
sec-Butylbenzene			11.72				
tert-Butylbenzene			11.50				
sec-Butyl butyrate			11.3				
Butyl chloroacetate			12.2				
Butyl 2-chlorobutyrate			12.6				
Butyl 3-chlorobutyrate			12.7				
Butyl 4-chlorobutyrate			13.0				
Butyl 2-chloropropionate			13.0				
Butyl 3-chloropropionate			13.3				
Butyl crotonate			12.4				
sec-Butyl crotonate			11.8				
Butylcyclohexane	3.384		11.96	66.00	93.10	112.30	125.70
Butylcyclopentane	2.704	9.20	11.00	57.77	80.38	97.35	114.80
N- Butyldiacetimide		8.69	15.4				
Butyl dichloroacetate			12.5				
tert- Butyl hydroperoxide			11.41				
Butylisobutylamine			10.73				
Butyl lithium			25.6				
Butyl trichloroacetate			12.8				
				1	T	1	1

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

				C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
1-Butyne	1.441		5.67	23.87	30.83	35.95	39.84
2-Butyne	2.207	5.861	6.38	22.62	29.68	35.14	39.29
Butyraldehyde	2.654	6.340	8.05	30.20	39.60	46.60	51.70
Butyric acid	2.50		15.2				
Butyronitrile	1.2	10.04	9.53	28.39	37.07	43.48	48.22
D-Camphor	1.635	8.13					
ε-Caprolactam		14.22	19.9				
Carbazole			20.2				
Carbon disulfide	1.049	6.401					
Chloroacetic acid			18				
Chloroacetyl chloride			9.3				
2-Chlorobenzaldehyde			13.3				
Chlorobenzene	2.28	8.73	9.81	30.62	41.16	47.89	52.48
2-Chlorobenzoic acid			19.0				
3-Chlorobenzoic acid			19.6				
4-Chlorobenzoic acid			21.0				
Chlorobenzoquinone			16.5				
1-Chlorobutane		7.38	8.0	32.30	42.77	50.31	55.92
2-Chlorobutane		6.98	7.60	32.52	43.18	50.84	56.60
Chlorocyclohexane			10.4				
Chlorodifluoromethane	0.985	4.833		15.63	18.87	20.84	22.10
Chloroethane	1.064	5.892		18.54	24.28	28.39	31.48
1-Chloro-2-ethylbenzene			11.3				
1-Chloro-4-ethylbenzene			11.5				
Chloroethylene				15.56	19.61	22.35	24.35
Chloroethyne				14.39	15.97	16.98	17.75
Chlorofluoromethane				13.29	16.57	18.81	20.39

Chloroform	2.28	7.08	7.48	17.75	20.38	21.87	22.83
Chloromethane	1.537	5.147	1	11.52	14.66	17.04	18.86
Chloromethyloxirane			9.7				
1-Chloro-2-methylpropane			7.57	32.52	43.18	50.84	56.60
2-Chloro-2-methylpropane	0.48	6.6		34.00	44.20	51.50	57.00
ΔHt , 0.41 at -90.1 °C; 1.39 at -53.6 °C							
1-Chloronaphthalene			15.6				
2-Chloronaphthalene			19.6				
1-Chloropentane		7.93	9.1	39.24	52.11	61.38	68.25
3-Chlorophenol			12.7				
4-Chlorophenol			12.4				
1-Chloropropane		6.62	6.9	25.36	33.43	39.24	43.59
2-Chloropropane		6.34	6.47	25.99	34.20	39.94	44.16
3-Chloro-1-propene				22.12	28.43	32.93	36.30
Chlorotrifluoromethane				18.53	21.60	23.17	24.03
Chlorotrinitromethane			10.86				
Chrysene			28.1				
o-Cresol		10.20	18.17	39.74	52.77	61.55	68.82
m-Cresol		10.32	14.75	38.74	52.26	61.27	68.50
p-Cresol		10.32	17.67	38.65	52.10	61.11	68.48
m-Cresyl acetate			14.51				
Cubane			19.2				
4-Cyanothiazole			17.67				
Cyclobutane ΔHt , 1.38 at -126.79 °C	0.260	5.781	5.65	23.89	34.76	42.42	47.96
Cyclobutene				21.59	30.30	36.26	40.53
Cyclododecane			18.26				
Cycloheptane ΔHt , 1.187 at -138.4 °C;	0.450	7.93	9.21	41.82	62.42	77.03	87.40
$0.069 \text{ at } -75.0 ^{\circ}\text{C}; 0.108 \text{ at } -60.8 ^{\circ}\text{C}$							
Cycloheptanone			12.4				
1,3,5-Cycloheptatriene ΔHt , 0.561 at -118.19 °C	0.277	9.250		37.13	50.07	58.58	64.58
Cyclohexane ΔHt , 1.611 at -87° C	0.640	7.160	7.896	35.82	53.83	66.76	75.80
Cyclohexanol ΔHt , 1.96 at -9.7 °C	0.406	10.875	12.820	41.14	59.29	72.18	81.13
Cyclohexanone		9.00	10.77	36.00	52.90	65.00	73.00
Cyclohexene ΔHt , 1.016 at -134.4 °C	0.787	7.285	8.00	34.64	49.45	59.49	66.62

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Cyclooctane ΔHt , 1.507 at -106.7 °C; 0.114 at -89.35 °C	0.576	8.58	10.36	47.82	71.00	87.30	99.01	
Cyclooctanone			13.0					
1,3,5,7-cyclooctatetraene	2.695	8.700	10.30	38.45	52.77	62.23	68.88	
Cyclopentadiene			6.78					
Cyclopentane ΔHt , 1.167 at -150.76 °C; 0.823 at -135.08 °C	0.1455	6.524	6.818	28.38	42.57	52.60	59.84	
Cyclopentanethiol	1.872	8.443	9.93	34.53	48.65	58.61	65.84	
Cyclopentanol			13.74					
Cyclopentanone			10.21					
Cyclopentene ΔHt , 0.115 at -186.08 °C	0.804		6.71	25.08	37.19	45.78	51.94	
Cyclopropane	1.301	4.793		18.31	26.15	33.57	35.39	
Decahydronaphthalene								
$cis \Delta Ht$, 0.511 at -57.1 °C	2.268	9.940	12.0	56.64	84.14	103.36	116.91	
trans	3.455	9.260	11.6	56.78	84.20	103.40	116.93	
Decanal				71.80	95.70	113.00	125.70	
Decane	6.863	9.388	12.277	71.24	96.36	114.92	128.20	
1-Decanethiol	7.4	11.1	15.5	76.63	102.63	122.10	136.98	
Decanoic acid	7.0		28.4					
1-Decanol	9.0	11.9	18.6	74.44	99.94	118.53	132.24	
1-Decene ΔHt , 1.90 at -74.8 °C	3.300	9.24	12.06	67.79	91.27	108.28	120.90	
1-Decyne				65.64	86.96	102.42	113.90	
Deoxybenzoin			22.3					
Dibenzilidene azine			22.3					
Dibenzyl ketone			21.3					
Dibenzyl sulfide			22.3					
Dibenzyl sulfone			27.8					

1,2-Dibromobutane			10.8	36.77	46.70	53.60	58.50
1,2-Dibromocycloheptane			12.43				
1,2-Dibromocyclohexane			12.07				
1,2-Dibromocyclooctane			13.04				
1,2-Dibromoethane	2.62	8.69	9.86	23.83	29.24	32.94	35.80
1,2-Dibromoheptane			13.01				
1,2-Dibromopropane				29.74	37.63	42.91	46.74
Dibutylborinic acid			15				
Dibutyl ether		8.83	10.5	60.78	81.29	96.52	107.86
Dibutyl mercury			15.6				
Di-tert-butyl peroxide			7.6				
Dibutyl o-phthalate			21.9				
Dibutyl sulfate			18.1				
Dibutyl sulfite			16.2				
Dibutyl sulfone			24.0				
Dichloroacetyl chloride			9.4				
1,2-Dichlorobenzene	3.19	9.7	11.56	34.12	44.07	50.28	54.42
1,3-Dichlorobenzene			11.44	34.18	44.09	50.29	54.42
1,4-Dichlorobenzene	4.34	9.5	15.5	34.24	44.16	50.35	54.46
2,6-Dichlorobenzoquinone			16.7				
2,2'-Dichlorobiphenyl			23.0				
4,4'-Dichlorobiphenyl			24.8				
Dichlorodifluoromethane				19.69	22.37	23.69	24.39
1,1-Dichloroethane	1.881	6.97	7.36	21.85	27.18	30.79	33.40
1,2-Dichloroethane	2.112	7.65	8.47	22.00	26.90	30.40	33.00
1,1-Dichloroethylene	1.557	6.26	6.328	18.80	22.44	24.71	26.29
1,2-Dichloroethylene							
cis	1.72	7.08	7.43	18.41	22.23	24.60	26.23
trans	1.72	6.65	6.92	18.58	22.28	24.62	26.24
Dichlorofluoromethane				16.78	19.70	21.41	22.51
Dichloromethane	1.1	6.74	6.94	14.24	17.30	19.32	20.76
1,2-Dichloropropane		7.59	8.68	28.60	36.47	41.97	46.08
1,3-Dichloropropane		8.10	9.66	28.69	36.22	41.56	45.50
2,2-Dichloropropane		7.0	7.8	30.56	38.06	43.00	46.56
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TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

				C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
Dicyanoacetylene			6.88				
2,2-Diethoxypropane			7.61				
Diethylamine			7.6	34.88	47.14	56.16	62.91
1,2-Diethylbenzene	4.01	9.42	12.61	56.01	75.66	89.54	99.49
1,3-Diethylbenzene	2.62	9.41	12.55	55.01	75.19	89.31	99.37
1,4-Diethylbenzene	2.53	9.41	12.54	54.68	74.84	89.04	99.16
Diethylene glycol		12.50	13.7				
Diethyl ether	1.745	6.38	6.516	33.01	43.92	52.26	58.51
Diethylmercury			10.7				
Diethylmethyl phosphonate			13.5				
Diethylnitramine			12.7				
Diethyl oxalate		10.04	15.2				
Diethyl peroxide			7.3				
Diethyl o-phthalate			21.1				
Diethyl selenide			9.3				
Diethyl sulfate			13.6				
Diethyl sulfite			11.6				
Diethyl sulfone			20.6				
Diethyl sulfoxide			14.9				
1,2-Difluorobenzene	2.640	7.699	8.65	32.76	43.33	50.12	54.72
1,3-Difluorobenzene			8.29	32.72	43.13	49.67	53.93
1,4-Difluorobenzene			8.51	32.84	43.20	49.68	53.99
2,2'-Difluorobiphenyl			22.7				
4,4'-Difluorobiphenyl			21.8				
1,1-Difluoroethane		5.1		19.93	25.70	29.70	32.57
1,1-Difluoroethylene				17.16	21.32	23.95	25.74
Difluoromethane				12.22	15.72	18.22	19.98

9,10-Dihydroanthracene			22.3	1			
4 <i>H</i> -Dihydropyran			7.7				
5,12-Dihydrotetracene			27.7				
2,3-Dihydrothiophene			9.02				
2,5-Dihydrothiophene			9.55				
1,2-Diiodobenzene			15.5				
1,2-Diiodoethane			15.7	22.94	27.92	31.37	33.84
Diiodomethane	3.02(I)		12.2	15.74	18.37	20.06	21.29
	2.88(II)						
Diisopropyl ether	2.635	6.95	7.75	46.90	62.61	74.39	83.17
Diisopropyl ketone			9.93				
Diisopropylmercury			12.8				
1,2-Dimethoxybenzene			16.0				
Dimethoxyborane			6.14				
2,2-Dimethoxypropane			7.03				
Dimethylamine	1.420	6.330	6.07	20.89	28.41	33.94	38.19
Dimethylaminotrimethylsilane			7.6				
2,2-Dimethylbutane ΔHt , 1.289 at	0.138	6.287	6.618	43.70	60.00	71.40	79.70
-147.34 °C; 0.068 at -132.28 °C							
2,3-Dimethylbutane ΔHt , 1.552 at	0.194	6.519	6.96	43.30	59.20	75.20	79.10
−137.08°C							
2,3-Dimethyl-1-butene		6.55	6.97	42.60	55.40	65.00	72.20
2,3-Dimethyl-2-butene a. ΔHt ,	1.542	7.083	7.776	37.48	51.78	62.78	71.14
b. 0.844 at – 76.34°C							
3,3-Dimethyl-1-butene ΔHt , 1.037 at	0.261	6.13	6.36	38.90	53.40	63.60	71.00
−148.3°C			0.05				
Dimethylcadmium	0.405		9.07	50.50	74.40	00.70	102.20
1,1-Dimethylcyclohexane Δ <i>Ht</i> , 1.430 at −120.01 °C	0.495	7.79	9.043	50.70	74.10	90.70	102.20
1,2-Dimethylcyclohexane							
cis ΔHt , 1.974 at -100.6 °C	0.393	8.04	9.492	51.10	74.00	90.10	101.40
trans	2.491(I)	7.86	9.168	51.90	74.60	90.50	101.70
er ceres	2.508(II)	7.00	7.100	31.50	7 1.00	70.50	101.70
1,3-Dimethylcyclohexane	2.000(11)						
cis	2.586	7.84	9.137	51.20	74.20	90.50	102.00
trans	2.358	8.09	9.369	51.10	73.80	89.80	101.10
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TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

				C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
1,4-Dimethylcyclohexane							
cis	2.225	8.07	9.329	51.10	73.80	89.80	101.10
trans	2.947	7.79	9.053	51.60	74.60	90.60	101.90
1,1-Dimethylcyclopentane	0.258	7.239	8.079	43.55	62.78	76.18	85.83
ΔHt , 1.551 at -126.36 °C							
1,2-Dimethylcyclopentane							
<i>cis</i> Δ <i>Ht</i> , 1.594 at −131.66°C	0.396	7.576	8.549	43.67	62.72	75.98	85.57
trans	1.713	7.375	8.259	43.71	62.66	75.84	85.43
1,3-Dimethylcyclopentane							
cis	1.761	7.265	8.200	43.71	62.66	75.84	85.43
trans	1.738	7.361	8.248	43.71	62.66	75.84	85.43
Dimethyldichlorosilane			8.2				
cis-2,4-Dimethyl-1,3-dioxane			9.53				
4,5-Dimethyl-1,3-dioxane			10.16				
5,5-Dimethyl-1,3-dioxane			9.86				
Dimethyl ether	1.180	5.141		19.02	25.16	30.04	33.79
N,N-Dimethylformamide			11.4				
Dimethylfulvene			10.6				
Dimethylglyoxime			23.2				
2,2-Dimethylhexane	1.62	7.71	8.91				
2,3-Dimethylhexane		7.94	9.27				
2,4-Dimethylhexane		7.79	9.03				
2,5-Dimethylhexane	3.096	7.80	9.05				
3,3-Dimethylhexane	1.7	7.76	8.97				
3,4-Dimethylhexane		7.95	9.32				
2,2-Dimethyl-3-hexene							
cis			8.88				
trans			8.91				

1,1-Dimethylhydrazine	1		8.37				
1,2-Dimethylhydrazine			9.40				
Dimethylmercury			8.26				
Dimethylnitramine			16.7				
2,2-Dimethylpentane	1.392	6.97	7.75	50.42	68.33	81.43	91.20
2,3-Dimethylpentane		7.26	8.19	50.42	68.33	81.43	91.20
2,4-Dimethylpentane	1.636	7.05	7.86	50.42	68.33	81.43	91.20
3,3-Dimethylpentane	1.689	7.09	7.89	50.42	68.33	81.43	91.20
2,7-Dimethylphenanthrene			25.5				
4,5-Dimethylphenanthrene			25.0				
9,10-Dimethylphenanthrene			28.6				
2,2-Dimethylpropane	0.752	5.438	5.205	37.55	51.21	60.78	67.80
ΔHt , 0.616 at -133.14 °C							
2,3-Dimethylpyridine			11.70				
2,4-Dimethylpyridine			11.42				
2,5-Dimethylpyridine			11.43				
2,6-Dimethylpyridine			11.01				
3,4-Dimethylpyridine			12.38				
3,5-Dimethylpyridine			12.04				
Dimethyl sulfate			11.6				
Dimethyl sulfite			9.6				
Dimethyl sulfone			18.4				
Dimethyl sulfoxide	1.56	12.66	12.64				
3,3-Dimethyl-2-thiabutane	2.011(I)	7.523	8.57				
	1.83(II)						
2,2-Dimethylthiacyclopropane			8.55				
2,2-Dimethyl-3-thiapentane	1.69	8.00	9.4				
2,4-Dimethyl-3-thiapentane	2.49	8.04	9.44	50.64	66.22	77.12	85.24
1,3-Dinitrobenzene			14.3				
2,4-Dinitrophenol			25				
2,6-Dinitrophenol			26.8				
1,1-Dinitropropane			14.93				
1,4-Dioxane ΔHt , 0.562 at -0.3 °C	3.07		9.20	30.23	43.44	52.15	58.05
1,3-Dioxolan			8.5				
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 TABLE 5.2
 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Dipentene			11.5					
Diphenylamine			23.1					
Diphenylchlorosilane			16.6					
Diphenyl disulfide			22.7					
Diphenyl disulfone			38.7					
1,2-Diphenylethane		12.3	20.1					
1,1-Diphenylethene			17.5					
Diphenyl ether	4.115	15.525	19.6					
Diphenylfulvene			25					
Diphenylmercury			26.95					
Diphenylmethane			19.7					
Diphenyl sulfide			16.2					
Diphenyl sulfone			25.4					
Diphenyl sulfoxide			23.2					
Dipropyl ether			8.6	46.90	62.61	74.39	83.17	
Dipropylmercury			13.2					
Dipropyl sulfate			16.0					
Dipropyl sulfite			14.0					
Dipropyl sulfone			19.1					
Dipropyl sulfoxide			17.8					
2,3-Dithiabutane	2.197	8.05	9.17	26.36	32.83	37.66	41.31	
5,6-Dithiadecane		11.2	15.2	68.38	89.98	105.83	117.86	
3,4-Dithiahexane	2.248	9.01	10.89	40.90	52.24	60.19	65.97	
1,3-Dithian-2-thione			21.85					
4,5-Dithiaoctane	3.30	10.02	12.55	44.50	71.30	83.70	93.20	
N,N-Dithiodiethylamine			12.6					
1,3-Diothiolan-2-thione			19.56					
Di-p-tolyl sulfone			26.2					

Divinyl ether			6.26		1		
Divinyl sulfone			13.5				
Dodecane	8.57	10.43	14.65	85.13	115.04	136.76	152.90
Dodecanedioic acid			36.6				
1-Dodecene	4.76	10.27	14.42	8.68	109.95	130.41	145.50
ΔHt , 1.088 at -60.2 °C							
Eicosane	16.70	13.74	24.1	140.65	189.78	225.28	251.60
Eicosanoic acid	17.2		48				
1-Eicosene	8.2	13.35	23.86	137.20	184.69	218.93	244.20
meso-Erythritol			32.3				
Ethane	0.683	3.517	1.200	15.65	21.35	25.81	29.30
1,2-Ethanedithiol			10.68				
Ethanethiol	1.189	6.401	6.526	21.08	27.21	31.83	35.38
Ethanol	1.198	9.255	10.11	19.36	25.69	30.33	33.83
Ethyl acetate	2.505	7.720	8.63	32.84	43.65	51.01	56.05
Ethyl allyl sulfone			20.0				
Ethylamine		6.7	6.7	21.65	28.68	33.89	37.88
N-Ethylaniline			12.5				
Ethylbenzene	2.195	8.50	10.10	40.76	56.44	67.15	74.77
3-Ethyl-1-butene		6.88	7.41	40.70	54.50	64.40	71.90
Ethyl crotonate			10.6				
Ethylcyclohexane	1.992	8.20	9.67	51.60	74.10	90.10	101.30
1-Ethylcyclohexene			10.34				
Ethylcyclopentane	1.642(I)	7.715	8.72	43.89	61.70	75.22	85.16
	1.889(II)						
Ethylene	0.801	3.237		12.67	17.87	20.03	22.43
Ethylene carbonate	2.41		17.5				
Ethylene glycol	2.78	11.86	15.68	27.06	32.72	36.90	39.88
Ethyleneimine		7.24	7.55	16.83	23.56	28.14	31.45
Ethylene oxide	1.236	6.101	5.96	14.95	20.62	24.60	27.47
Ethyl formate	2.20	7.201					
2-Ethyl-1-hexanal			11.70				
3-Ethylhexane		8.03	9.48				
Ethylisovalerate			10.5				
Ethyllithium			27.9				

 TABLE 5.2
 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C _p 800 K 1000 K				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Ethylmercury bromide			18.3					
Ethylmercury chloride			18.2					
Ethylmercury iodide			19.0					
Ethyl methyl ether	2.04	7.02	0.67	26.08	34.58	41.19	46.18	
Ethyl nitrate	2.04	7.92	8.67 8.42	28.73	37.07	42.72	46.69	
3-Ethylpentane Ethyl pentanoate	2.282	7.40	11.0	50.42	68.33	81.43	91.20	
2-Ethylphenol			15.20					
3-Ethylphenol			16.30					
4-Ethylphenol			19.20					
Ethylphosphonic acid			12.1					
Ethyl propanoate		8.178	9.0					
Ethyl β-vinylacrylale			11.6					
Ethyl vinyl ether			6.35					
Ethynylbenzene				35.95	48.01	55.79	61.17	
Fluoranthrene			24.65					
Fluorobenzene	2.702	7.457	8.27	29.99	40.86	47.83	52.58	
4-Fluorobenzoic acid			21.8					
Fluoroethane				17.71	23.56	27.82	31.00	
Fluoromethane				10.56	13.83	16.45	18.44	
1-Fluoropropane				24.55	32.82	38.88	43.37	
2-Fluoropropane				24.72	33.14	39.14	43.55	
4-Fluorotoluene	2.235	8.144	9.42	36.43	49.70	58.60	64.84	
Fluorotrinitromethane			8.3					
Formaldehyde		5.85		9.38	11.52	13.37	14.81	
Formic acid	3.035	5.24	11.03	12.85	16.02	18.35	19.95	
Formyl				0.72	0.70	10.75	11.40	
HCO·				8.73	9.79	10.75	11.49	
HCO ⁺			I	9.39	10.39	11.14	11.78	

Fumaric acid			32.5				
Funaronitrile	0.909	6.474	17.2 6.61	21.20	20.21	24.41	37.89
Furan ΔHt , 0.489 at -123.2 °C	3.12	0.4/4	15.4	21.20	29.31	34.41	37.89
Furfuryl alcohol 2-Furoic acid	5.12		25.92				
Furylethylene			9.1				
, ,							
Glycerol	4.416		20.5				
Glyceryl triacetate			19.6				
Glyceryl trinitrate			23.9				
Heptadecane ΔHt , 2.62 at 11.1 °C	9.67	12.64	20.6	119.83	161.75	192.08	214.60
Heptadecanoic acid	12.3						
1-Heptadecene	7.5	12.39	20.32	116.38	156.66	185.74	207.20
1-Heptanal	5.637		11.40	51.00	67.70	79.80	88.70
Heptane	3.359	7.575	8.74	50.42	68.33	81.43	91.20
1-Heptanethiol	6.067	9.5	12.06	55.81	74.60	88.91	99.98
Heptanoic acid			18.0				
1-Heptanol	3.16	11.5	16.5	53.62	71.92	85.32	95.25
1-Heptene ΔHt , 0.07 at 1.36°C	2.964(I) 3.021(II)	7.43	8.52	46.97	63.24	75.09	83.90
Hexachlorobenzene	6.1		23.2	48.08	55.78	59.96	62.34
Hexachloroethane ΔHt , 1.9 at 71.3 °C	2.33	12.2	16.5	36.21	39.82	41.48	42.38
Hexadecafluoroethylcyclohexane			9.20				
Hexadecafluoroheptane			8.7				
Hexadecane	12.39	12.24	19.38	112.89	152.41	181.02	202.20
Hexadecanoic acid	12.8		36.9				
1-Hexadecanol Δ <i>Ht</i> , 4.8 at 44.0 °C; 5.7 at 49.1 °C	7.8		40.5	116.09	156.00	184.90	206.30
1-Hexadecene	7.216	12.05	19.14	109.44	147.32	174.67	194.80
Hexafluorobenzene	2.770	7.571	8.61	43.88	52.55	57.62	60.63
Hexafluoroethane ΔHt , 0.893 at -169.17 °C	0.642	3.860		30.01	35.60	38.40	39.87
Hexahydroindane							
cis			11.0				
trans			10.7				
ишь	1		10.7	T.	1		

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
Hexamethylbenzene ΔHt , 0.269 at -156.67 °C; 0.422 at 110.7 °C	4.93		17.9	74.18	97.13	113.51	125.55	
Hexmethyldisiloxane Hexanal Hexanamide			8.9 22.72	44.00	58.30	68.70	76.40	
Hexane 1-Hexanethiol	3.126 4.305	6.896 8.9	7.54 11.14	43.47 48.87	58.99 65.26	70.36 77.84	78.89 87.65	
Hexanoic acid 1-Hexanol	6.98 3.68	15.45 11.6	17.3 14.8	46.68	62.58	74.25	82.92	
1-Hexene 2-Hexene	2.234	6.76	7.32	40.03	53.90	64.02	71.54	
cis trans 3-Hexene		6.96 6.91	7.52 7.54	38.60 39.70	53.00 53.40	63.40 63.60	71.20 71.20	
cis trans 1-Hexyne		6.86 6.92	7.47 7.54	38.50 40.20 37.87	53.20 53.90 49.59	63.50 63.90 58.16	71.20 71.40 64.56	
Hydroquinone 8-Hydroxyquinoline			23.7 26.0					
Indane Indene Indole			11.8 12.64 16.7					
Iodobenzene 4-Iodobenzoic acid Iodocyclohexane	2.33	9.44	11.85 21.0 11.3	31.10	41.43	48.07	52.60	
Iodoethane Iodomethane		7.115 6.52	7.7 6.63	19.18 12.33	24.64 15.28	28.65 17.47	31.65 19.17	

	2-Iodo-2-methylpropane	3.47	I	8.46	35.27	45.82	52.85	57.91
	1-Iodonaphthalene			17.3				
	2-Iodonaphthalene			21.7				
	1-Iodopropane			8.6	26.27	34.11	39.80	44.03
	2-Iodopropane			8.14	26.59	34.58	40.21	44.34
	3-Iodopropene			9.1				
	Iodotoluene, 3- and 4-			13.0				
	Isobutylbenzene			11.54				
	Isobutyl dichloroacetate			12.5				
	Isobutyl phenyl ketone			14.22				
	Isobutyl trichloroacetate			12.7				
	Isobutyronitrile	7.754	8.99	28.56	37.39	43.74	48.40	
	Isopropyl acetate			8.89				
	Isopropylbenzene	1.86	8.97	10.79	48.00	66.20	78.60	87.30
	Isopropyl nitrate		8.35	9.27	35.96	46.81	54.13	59.26
	Isopropyl trichloroacetate			12.4	10.51			4 6 5 5
	Isothiocyanic acid				12.71	14.57	15.74	16.57
	Ketene			4.18	14.22	16.89	18.80	20.25
	Lauric acid	8.8		31.7				
	Leucine			36.0				
	(+)-Limonene			11.5				
	Maleic acid			26.3				
	Maleic anhydride			17.1				
	Malononitrile			18.9				
	D-Mannitol	5.39						
	Melamine			29.7				
	2,2-Metacyclophane			22.0				
	Methane	0.225	1.953		9.71	12.55	15.18	17.40
	ΔHt , 0.0187 at -248 to -252.7 °C							
	Methanethiol ΔHt , 0.0525 at -135.6 °C	1.411	5.872	5.7	14.04	17.57	20.32	22.48
	Methanol ΔHt , 0.152 at -115.8 °C	0.768	8.24	8.94	12.29	16.02	19.04	21.38
បា	4-Methoxybenzaldehyde			15.42				
5.61	Methoxybenzene			11.18				
	2-Methoxytetrahydropyran			10.2				
	Methyl (CH ₃)				10.05	11.54	12.89	14.09

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
Methyl allyl sulfone			19.0				
Methylamine	1.466	6.169	5.80	14.38	18.86	22.44	25.26
Methyl benzyl sulfone			23.7				
2.Methyl-1,3-butadiene	1.155	6.191	6.32	31.80	41.40	48.00	52.90
3-Methyl-1,2-butadiene		6.51	6.68	31.00	40.30	47.20	52.40
2-Methylbutane	1.231	5.901	5.94	36.49	49.89	59.71	67.12
2-Methyl-1-butanethiol		8.0					
3-Methyl-1-butanethiol	1.78						
2-Methyl-2-butanethiol	0.1454	7.50	8.51	42.79	56.58	66.28	73.30
ΔHt , 1.907 at -114.0° C							
3-Methylbutanoic acid	1.750	10.32					
2-Methyl-1-butanol		10.5	12.9				
3-Methyl-1-butanol		10.54	13.0				
2-Methyl-2-butanol	1.06	9.6	11.9				
ΔHt , 0.47 at -127.2 °C							
3-Methyl-2-butanol		9.9	12.4				
2-Methyl-1-butene	1.891	6.094	6.181	33.20	44.72	53.15	59.43
3-Methyl-1-butene	1.281	5.750	5.70	35.26	45.90	53.85	59.83
2-Methyl-2-butene	1.816	6.287	6.468	31.93	43.42	52.05	58.55
Methyl butyl sulfone			18.2				
Methyl tert-butyl sulfone			19.7				
3-Methyl-1-butyne		6.25	6.16	31.10	40.60	47.40	52.40
Methyl crotonate			9.8				
Methylcyclohexane	1.614	7.44	8.45	44.35	64.46	78.74	88.79
2-Methylcyclohexanol, cis- and trans-			15.1				
3-Methylcyclohexanol							
cis			15.6				
trans			15.7				

4-Methylcyclohexanol		1		1			
cis			15.7				
trans			15.8				
Methylcyclopentane	1.656	6.95	7.55	36.11	52.43	64.00	72.44
1-Methylcyclopentene			7.55	32.50	46.80	57.00	64.30
3-Methylcyclopentene			7.7	32.60	47.10	57.20	64.50
4-Methylcyclopentene			7.7	32.60	47.00	57.10	64.40
Methyldichlorosilane			6.7				
2-Methyl-1,3-dioxane			9.23				
4-Methyl-1,3-dioxane			9.36				
Methylene (CH ₂)				8.64	9.37	10.14	10.89
1-Methyl-2-ethylbenzene	2.38	9.29	11.40	48.50	65.80	78.10	86.90
	2.28						
1-Methyl-3-ethylbenzene	1.82	9.21	11.21	47.50	65.40	77.80	86.80
	1.79						
1-Methyl-4-ethylbenzene	3.19	9.18	11.14	47.20	65.00	77.60	86.60
2-Methyl-3-ethylpentane	2.71	7.88	9.20				
3-Methyl-3-ethylpentane	2.59	7.84	9.08				
2-Methyl-3-ethyl-1-pentene			8.98				
Methyl ethyl sulfite			10.4				
Methyl ethyl sulfone			18.6				
Methyl formate	1.800	6.75		19.50	25.20	29.10	32.00
Methylglyoxal			9.1				
2-Methylheptane	2.839	8.08	9.48				
3-Methylheptane	2.779	8.10	9.52				
4-Methylheptane	2.59	8.10	9.48				
Methyl heptanoate			12.0				
2-Methylhexane	2.195	7.33	8.32	50.42	68.33	81.43	91.20
3-Methylhexane		7.36	8.39	50.42	68.33	81.43	91.20
Methyl hexanoate			11.1				
Methylhydrazine			9.65				
Methylidyne							
СН				6.98	7.11	7.40	7.78
CH ⁺				6.98	7.10	7.36	7.65
1-Methyl-2-isopropylbenzene	2.39	9.17	12.10				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

				C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
1-Methyl-3-isopropylbenzene	3.27	9.11	11.94					
1-Methyl-4-isopropylbenzene	2.31	9.12	12.02					
Methyl isopropyl ether			6.27	32.97	44.17	52.67	59.08	
Methyl isopropyl ketone			8.82					
Methyl isopropyl sulfone			16.8					
3-Methylisoxazole			9.8					
5-Methylisoxazole			10.0					
Methylmercury bromide			16.2					
Methylmercury chloride			15.5					
Methylmercury iodide			15.6					
1-Methylnaphthalene	1.160	11.0		50.74	69.79	82.48	91.21	
ΔHt , 1.190 at -32.37 °C								
2-Methylnaphthalene	2.808	11.0		50.50	69.31	82.03	90.86	
ΔHt , 1.34 at 15.4°C								
Methyl nitrate	1.97	7.54	8.1	21.87	27.54	31.47	34.19	
Methyl nitrite		5.0	5.4	18.24	23.35	26.97	29.52	
2-Methylpentane	1.498	6.643	7.138	44.00	59.60	70.80	79.20	
3-Methylpentane		6.711	7.236	43.47	59.00	70.40	78.90	
Methyl pentanoate			10.2					
2-Methyl-1-pentene		6.71	7.29	40.80	54.40	64.40	71.80	
3-Methyl-1-pentene		6.43	6.83	42.50	55.60	65.20	72.30	
4-Methyl-1-pentene		6.47	6.86	38.90	52.90	63.10	70.70	
2-Methyl-2-pentene		6.93	7.55	39.00	53.20	58.60	71.10	
3-Methyl-2-pentene								
cis		6.89	7.49	39.00	53.20	63.40	71.10	
trans		7.00	7.67	39.00	53.20	63.40	71.10	
4-Methyl-2-pentene								
cis		6.59	7.04	40.05	54.10	64.00	71.50	
trans		6.68	7.16	41.90	54.80	64.50	71.80	

Methyl phenyl sulfone			22.0				1
Methylphosphonic acid			11.5				
2-Methylpropanal			7.5				
2-Methylpropane	1.085	5.089	4.57	29.77	40.62	48.49	54.40
2-Methyl-1-propanethiol	1.191	7.412	8.28	35.31	46.26	53.77	59.17
2-Methyl-2-propanethiol							
ΔHt , 0.972 at -121.6 °C;	0.593	6.80	7.36	36.13	47.60	55.53	61.24
$0.155 \text{ at} - 116.2 ^{\circ}\text{C}; 0.232 \text{ at} - 73.8 ^{\circ}\text{C}$							
2-Methyl-1-propanol		9.80	12.04				
2-Methyl-2-propanol	1.602	9.33	12.73	34.16	45.37	53.28	59.16
ΔHt , 0.20 at 12.99 °C							
2-Methylpropene	1.418	5.286	4.92	26.57	35.30	41.86	46.85
Methyl propyl ether			6.6	33.01	43.92	52.26	58.51
2-Methylpyridine	2.324	8.654	10.15	31.92	44.55	53.21	59.34
3-Methylpyridine	3.389	8.932	10.62	31.82	44.47	53.12	59.23
α -Methylstyrene				44.80	60.70	71.80	79.80
β -Methylstyrene							
cis				44.80	60.70	71.80	79.80
trans				45.20	61.20	72.20	80.00
3-Methyl-2-thiabutane	2.236	7.338	8.15	34.69	46.01	54.95	62.29
2-Methylthiacyclopentane		8.7	10.1				
2-Methyl-3-thiapentane	2.08		9.2				
4-Methylthiazole			10.48				
2-Methylthiophene	2.263	8.103	9.26	29.43	39.57	46.43	51.30
3-Methylthiophene	2.518	8.186	9.44	29.38	39.34	45.95	50.59
Naphthalene	4.536	10.34	17.6	42.83	59.67	70.77	78.38
1-Naphthol		10.51	21.9	12.00	25.07	, , , , ,	, 0.50
2-Naphthol			19.8				
1,4-Naphthoquinone			17.3				
1-Naphthylamine			21.5				
2-Naphthylamine			21.1				
p-Nitroaniline	5.04		26				
Nitrobenzene	2.78	9.744					
1-Nitrobutane		9.3	11.6	37.65	50.21	59.03	65.39
2-Nitrobutane		8.8	10.48	37.61	50.46	59.44	65.96
	1	1	1	1	1	1	1

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

					C_p			
Substance	ΔHm	ΔHv	ΔHs	400 K	600 K	800 K	1000 K	
Nitroethane		8.4	9.9	23.66	31.45	36.81	40.67	
Nitromethane	2.319	8.12	9.17	16.80	21.92	25.56	28.17	
1-Nitronaphthalene			25.6					
1-Nitropropane		8.8	10.37	30.72	40.87	47.96	53.06	
2-Nitropropane		8.4	9.88	30.89	41.19	48.22	53.24	
Nonadecane ΔHt , 3.30 at 22.8 °C	10.95	13.39	22.9	133.71	180.43	214.21	239.20	
1-Nonadecene	8.0	13.06	22.68	130.26	175.35	207.86	231.80	
1-Nonanal			17.28	64.80	86.40	101.90	113.40	
Nonane ΔHt , 1.50 at -55.97 °C	3.72	8.82	11.10	64.30	87.01	103.56	115.90	
1-Nonanethiol	8.0	10.6		69.69	93.28	111.04	124.65	
Nonanoic acid			19.7					
1-Nonanol		13.0	18.6	67.50	90.60	107.46	119.91	
1-Nonene	4.3	8.68	10.88	60.85	81.93	97.22	108.50	
Octadecane	14.81	13.02	21.7	126.77	171.09	203.15	226.90	
Octadecanoic acid	15.1		39.8					
1-Octadecene	7.8	12.74	21.50	123.32	166.00	196.80	219.50	
Octafluorocyclobutane	0.662	5.58		44.50	53.85	58.65	61.50	
1-Octanal			16.28	57.90	77.00	90.90	101.00	
Octanamide			26.4					
Octane	4.957	8.225	9.916	57.35	77.67	92.50	103.60	
1-Octanethiol	58	10.1		62.75	83.94	99.97	112.31	
Octanoic acid	3.30	16.73	19.2					
1-Octanol	10.1	11.2	15.6	60.56	81.26	96.39	107.58	
1-Octene	3.660	8.07	9.70	53.91	72.58	86.15	96.20	
1-Octyne				51.75	68.28	80.30	89.20	
Oxalic acid ΔHt , $0.3(\alpha \rightarrow \beta)$			23.4					
Oxalyl chloride			7.6					
Oxamide			26.8					

Palmitic acid	10.30		37				
[1.8]-Paracyclophane			26.5				
[2.2]-Paracyclophane			23.0				
[6.6]-Paracyclophane			27.5				
Paraldehyde			9.9				
Pentachloroethane	2.7	8.9	10.9	31.96	36.35	38.71	40.17
Pentachlorofluoroethane	0.449						
Pentachlorophenol			16.1				
Pentadecane ΔHt , 2.19 at -2.25 °C	8.31	11.82	18.20	105.95	143.07	169.95	189.90
1-Pentadecene	6.9	11.63	17.96	102.50	137.98	163.60	182.50
1.2-Pentadiene		6.59	6.85	31.40	40.80	47.70	52.80
1.3-Pentadiene							
cis		6.60	6.77	29.50	39.90	47.00	52.20
trans		6.46	6.64	31.20	40.90	47.70	52.60
1.4-Pentadiene	1.468	6.01	6.01	31.30	40.80	47.60	52.70
2,3-Pentadiene		6.75	7.05	29.90	39.40	46.60	52.00
Pentaerythritol		0.75	34.4	25150	370		52.00
Pentaerythritol tetranitrate			36.3				
Pentafluorobenzoic acid			21.9				
Pentafluoroethane				27.20	32.94	36.12	37.98
Pentafluorophenol			16.1		0 = 1,7		
Pentamethylbenzene	2.95		10.1	65.00	86.08	101.29	112.33
ΔHt , 0.473 at 23.7°C	2.50			02.00	00.00	101.29	112.00
1-Pentanal				37.10	49.00	57.70	64.00
Pentanamide			21.34	57.10	.,,,,,	37170	00
Pentan-2,4-dione			10.82				
Pentane	2.008	6.16	6.32	36.53	49.64	59.30	66.55
Pentan-1,5-dithiol	2.000	0.10	14.17	30.33	15.01	37.50	00.55
Pentanenitrile	1.130	7.98	11.17				
1-Pentanethiol	4.19	8.34	9.83	41.93	55.92	66.78	75.32
Pentanoic acid	3.850	10.53	16.6	41.73	33.72	00.70	75.52
1-Pentanol	2.34	10.6	13.61	39.74	53.24	63.18	70.59
2-Pentanol	2.34	10.3	12.7	37.74	33.24	05.10	70.57
3-Pentanol		10.1	12.8				
2-Pentanone		7.98	9.89	36.42	48.32	57.13	63.61

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

				C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K	
1-Pentene	1.388	6.02	6.09	33.10	44.56	52.95	59.21	
2-Pentene								
cis	1.700	6.24	6.41	31.57	43.62	52.29	58.78	
trans	1.996	6.23	6.38	32.67	44.02	52.45	58.81	
1-Pentyne		6.63	6.79	31.10	40.40	47.10	52.20	
2-Pentyne		6.99	7.35	29.20	38.70	45.90	51.40	
Perylene			30.0					
α -Phellandrene			12.1					
9,10-Phenanthraquinone			21.9					
Phenanthrene		13.3	21.1					
Phenol	2.752	9.73	16.41	32.45	43.54	50.62	55.49	
Phenyl acetate			13.0					
β-Phenyl-1-alanine, DL- and L-			36.8					
Phenyl benzoate			23.0					
N-Phenyldiacetimide			21.5					
Phenyl ethyl sulfide			13.2					
Phenylhydrazine			14.69					
1-Phenyl-2-methylpropane	2.99	9.04	11.82					
Phenyl methyl sulfide			12.1					
Phenyl salicylate			22.0					
Phosgene	1.372	5.832		15.28	16.98	17.92	18.49	
-	1.335							
	1.131							
m-Phthalic acid			25.5					
p-Phthalic acid			23.5					
Phthalic anhydride			21.19					
α -Pinene			10.7					
α-Pinene			10.7					

β -Pinene			11.1				1
Propadiene		4.45		17.21	22.00	25.42	28.00
1-Propanal			7.09	23.09	30.22	35.45	39.27
Propane	0.842	4.487	3.605	22.47	30.76	36.99	41.73
Propane-2,3-dithiol			11.87				
1-Propanethiol ΔHt , 0.949 at -131.06 °C	1.309	7.059	7.62	27.86	36.72	43.60	49.01
2-Propanethiol ΔHt , 0.013 at -160.6 °C	1.371	6.670	7.039	28.35	37.02	43.26	47.92
1-Propanol	1.242	9.982	11.36	25.86	34.56	41.04	45.93
2-Propanol	1.293	9.510	10.85	26.78	35.76	42.13	46.82
2-Propen-1-ol			11.3	22.81	30.11	35.28	39.06
Propionic acid	1.800	7.716	13.7				
Propionic anhydride			12.6				
Propionitrile ΔHt , 0.408 at -96.19 °C	1.202	7.353	8.632	21.18	27.42	32.14	35.70
1-Propylamine			7.46	28.51	37.99	44.94	50.21
Propylbenzene	2.215	9.14	11.05	47.82	65.86	78.30	87.16
	2.03						
Propyl carbamate			19.4				
Propyl chloroacetate			11.6				
Propylcyclohexane	2.479	8.62	10.78	59.10	83.80	101.20	113.40
Propylcyclopentane	2.398	8.15	9.82	50.83	71.04	86.28	97.50
Propylene	0.718	4.40		19.23	25.81	30.77	34.52
Propylene oxide	1.561	6.87	6.67	22.16	30.07	35.68	39.79
Propyl nitrate		8.58	9.70	35.79	46.49	53.87	59.08
Propyl phenyl ketone			14.51				
Propyl trichloroacetate			12.7				
Propyne		5.29		17.33	21.80	25.14	27.71
Pyrazine			13.45				
Pyrene			22.5				
Pyridazine			12.78				
Pyridine	1.979	8.39	9.61	25.42	35.72	42.49	47.17
Pyrimidine			11.95				
Pyrrole			10.80				
Pyrrolidine ΔHt , 0.129 at -66.01 °C	2.050	7.89	8.98	27.33	40.31	49.35	55.84
Salicyclic acid			22.74				
Sebacic acid			38.4				
		I .	1	1	1	1	1

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

					C_p				
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K		
5,5'-Spirobis(1,3-dioxane)			17.4						
Spiropentane	1.538	6.39	6.58	28.55	40.10	47.91	53.51		
cis-Stilbene			16.5						
Styrene	2.617	8.85	10.50	38.32	52.14	61.40	67.92		
Suberic acid			34.2						
Succinic acid			28.1						
Tetrabromomethane				23.20	24.51	25.51	25.32		
Tetracene			30						
Tetrachlorobenzoquinone			23.6						
1,1,1,2-Tetrachloroethane				28.36	33.28	36.24	38.17		
1,1,2,2-Tetrachloroethane		9.24	10.7	27.90	32.91	35.85	37.76		
Tetrachloroethylene	2.5	8.3	9.4	25.10	27.86	29.29	30.07		
Tetrachloromethane									
ΔHt , 1.095 at -47.9 °C	0.601	7.16	7.79	21.92	23.82	24.64	25.05		
Tetracyanoethylene			19.4						
Tetradecane	10.90	11.38	17.01	99.01	133.72	158.89	177.60		
Tetradecanoic acid			33.4						
1-Tetradecene	6.6	11.21	16.78	95.56	128.64	152.54	170.20		
Tetraethylene glycol			24						
Tetraethyllead			13.6						
1,1,1,2-Tetrafluoroethane				24.90	30.76	34.20	36.36		
Tetrafluoroethylene	1.844	4.02		21.97	25.53	27.61	28.86		
Tetrafluoromethane									
ΔHt , 0.353 at -196.92 °C	0.167			17.30	20.74	22.58	23.61		
Tetrahydrofuran			7.65						
Tetrahydrofurfuryl alcohol			15.9						
1,2,3,4-Tetrahydronaphthalene			13.4						
Tetrahydropyran			8.35						

Tetraiodomethane				24.00	24.94	25.31	25.49
1,2,3,4-Tetramethylbenzene	2.684	10.76	13.66	56.81	75.68	89.42	99.47
1,2,3,5-Tetramethylbenzene	2.561	10.47	13.34	55.76	74.81	88.79	99.01
1,2,4,5-Tetramethylbenzene	5.02	10.88	18	55.50	74.38	88.41	98.71
2,2,3,3-Tetramethylbutane	1.802	7.51	10.24				
ΔHt , 0.478 at -120.66 °C							
Tetramethyllead			9.1				
Tetranitromethane			10.3				
Tetrazole			23				
2-Thiabutane	2.333	7.06	7.61	27.81	36.41	42.93	47.94
Thiacyclobutane							
ΔHt , 0.160 at -96.45 °C	1.971	7.7	8.56	21.89	30.45	36.40	40.67
Thiacycloheptane			11.30	42.0	65.0	79.0	88.0
Thiacyclohexane							
ΔHt , 0.262 at -71.75 °C;	0.585	8.60	10.22	35.71	52.37	64.00	72.34
$1.858 \text{ at } -33.14 ^{\circ}\text{C}$							
Thiacyclopentane	1.757	8.28	9.28	28.95	40.04	47.66	53.14
Thiacyclopropane		6.98	7.24	16.53	21.99	25.61	28.21
4-Thia-5,5'-dimethyl-1-hexene			10.6				
2-Thiaheptane			10.88	48.67	65.02	77.59	87.41
3-Thiaheptane	2.96	8.78	10.74	48.37	64.96	77.74	87.75
4-Thiaheptane	2.90	8.76	10.64	48.21	65.13	78.45	89.05
2-Thiahexane	2.976	8.2	9.8	41.73	55.68	66.53	75.08
3-Thiahexane	2.529	8.3	9.58	41.43	55.62	66.68	75.42
5-Thianonane	4.64		12.75	62.09	83.81	100.58	113.71
2-Thiapentane	2.369	7.62	8.65	34.64	45.86	54.45	61.14
3-Thiapentane	2.845	7.59	8.55	34.65	46.11	54.91	61.79
2-Thiapropane	1.908	6.45	6.61	21.12	27.01	31.58	35.17
6-Thiaundecane			14.7				
Thioacetic acid				22.25	26.72	30.41	32.62
Thiophene ΔHt , 0.152 at -101.6 °C	1.216	7.52	8.27	23.02	30.95	36.01	39.54
Thymol			21.8				
Toluene	1.586	7.93	9.08	33.48	47.20	56.61	63.32
2-Toluenethiol			12.3				
2,4,6-Triamino-1,3,5-triazine			29.5				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
Tribromomethane				18.80	21.03	22.29	23.12
Tributyl phosphate			17.2				
Trichloroacetyl chloride			9.8				
Trichlorobenzoquinone			21.2				
1,1,1-Trichloroethane							
ΔHt , 1.79 at -48.95 °C	0.45	7.96	7.76	25.72	30.68	33.73	35.81
1,1,2-Trichloroethane	2.7	8.3	9.4	25.03	30.13	33.28	35.42
Trichloroethylene		7.52	8.2	21.80	25.06	26.94	28.15
Trichlorofluoromethane				20.84	23.13	24.19	24.74
Trichloromethyl (CCl ₃)				16.66	18.16	18.83	19.18
1,2,3-Trichloropropane		8.87	11.22	31.71	38.87	43.79	47.34
Tricyanoethylene			19.4				
Tridecane ΔHt , 1.831 at -18.2 °C	6.81	10.91	15.83	92.07	124.38	147.82	165.20
Tridecanoic acid	8.2		35.0				
1-Tridecene	6.2	10.75	15.60	88.62	119.29	141.48	157.80
Trimethylaluminum			17.5				
Triethylamine			8.29	48.70	66.10	78.56	87.80
Triethylaminoborane			14.5				
Triethyl arsenite			12.1				
Triethylarsine			10.3				
Triethyl borate			10.5				
Triethylenediamine							
ΔHt , 2.30 at 79.8 °C	1.45		14.8				
Triethylene glycol		17.07	18.9				
Triethyl phosphate			13.7				
Triethylphosphine			9.5				
Triethyl phosphite			10.0				
Triethylstibine			10.4				

1,1,1-Trifluoroethane	1.480	4.58		22.75	28.38	31.98	34.44
Trifluoroethylene				19.39	23.30	25.69	27.23
Trifluoromethane	0.970	3.99		14.61	18.16	20.35	21.76
Trifluoromethyl							
CF_2				13.74	16.17	17.50	18.25
CF ₃ ⁺				13.62	16.00	17.35	18.13
Trifluoromethylbenzene	3.29	7.80	8.98	40.59	54.20	62.75	68.45
Triodomethane	3.9		16.7	19.60	21.52	22.64	23.38
2,4,5-Trimethylacetophenone			15.1				
2,4,6-Trimethylacetophenone			14.9				
Trimethylaluminum			15.1				
Trimethylamine	1.564	5.48	5.26	28.08	38.34	45.62	50.98
Trimethyl arsenite			10.1				
Trimethylarsine			6.9				
1,2,3-Trimethylbenzene	1.955	9.57	11.73	46.90	64.00	76.70	85.90
ΔHt , 0.157 at -54.46 °C;							
$0.319 \text{ at } -42.89 ^{\circ}\text{C}$							
1,2,4-Trimethylbenzene	3.153	9.38	11.46	46.96	64.29	76.93	86.10
1,3,5-Trimethylbenzene	2.274	9.33	11.35	46.41	64.08	76.84	86.07
·	1.932						
	1.892						
Trimethyl borate			8.3				
Trimethylboron			4.83				
2,2,3-Trimethylbutane							
ΔHt , 0.586 at -157.8 °C	0.540	6.92	7.65	50.83	69.61	82.73	92.32
Trimethylchlorosilane			7.2				
cis, cis-1,3,5-Trimethylcyclohexane				58.05	83.94	102.20	115.21
2,2,3-Trimethylpentane	2.06	7.65	8.82				
2,2,4-Trimethylpentane	2.20	7.41	8.40				
2,3,3-Trimethylpentane	0.205	7.73	8.90				
ΔHt , 1.850 at -109.01 °C							
2,3,4-Trimethylpentane	2.215	7.82	9.01				
2,4,4-Trimethyl-1-pentene		7.5	8.5				
2,4,4-Trimethyl-2-pentene		7.8	8.9				
Trimethylphosphine			6.7				
Trimethylphosphine oxide			12.0				
√ 1 1	1	I	1	T. Control of the Con	1	1	1

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (continued)

				C_p			
Substance	ΔHm	$\Delta H v$	ΔHs	400 K	600 K	800 K	1000 K
Trimethyl phosphite			8.8				
Trimethylsilanol			10.9				
Trimethylstibine			7.5				
Trimethylsuccinic anhydride			17.7				
Trimethylthiacyclopropane			9.40				
2,4,6-Trinitroanisole			31.8				
1,3,5-Trinitrobenzene			23.8				
Trinitromethane			11.15				
2,4,6-Trinitrophenetole			28.8				
2,4,6-Trinitrotoluene			28.3				
Triphenylarsine			23.5				
Triphenylene			28.2				
Triphenylmethane			23.9				
Triphenylphosphine			23				
Tropolone			20.0				
Undecane ΔHt , 1.64 at -36.55 °C	5.28	9.92	13.47	78.18	105.80	125.69	140.60
Undecanoic acid	6.2		29.0				
1-Undecene ΔHt , 2.202 at -55.8 °C	4.06	9.77	13.24	74.74	100.61	119.34	133.20
Urea			21.0				
o- Xylene	3.25	8.80	10.38	41.03	55.98	66.64	74.35
m-Xylene	2.765	8.69	10.20	40.03	55.51	66.41	74.23
<i>p</i> -Xylene	4.09	8.60	10.13	39.70	55.16	66.14	74.02
2,3-Xylenol	4.02	0.00	20.1	37.70	33.10	00.14	74.02
2,4-Xylenol			15.74				
2,5-Xylenol			20.31				
2,6-Xylenol			18.07				
3,4-Xylenol			20.49				
3,5-Xylenol			19.80				
5,5-Ayichoi			17.00				

CRITICAL PHENOMENA

The *critical temperature* T_c of a gas is the temperature above which the gas cannot be liquefied no matter how high the pressure.

The *critical pressure* P_c is the lowest pressure which will liquefy the gas at its critical temperature.

The critical molar volume V_c is the volume of 1 mol at the critical temperature and the critical pressure. It can be computed from the critical density ρ_c as follows:

$$\frac{\text{Molecular weight in g} \cdot \text{mol}^{-1}}{\rho_c \text{ in g} \cdot \text{cm}^{-3}} = V_c \text{ in cm}^3 \cdot \text{mol}^{-1}$$

The critical pressure, critical molar volume, and critical temperature are the values of the pressure, molar volume, and thermodynamic temperature at which the densities of coexisting liquid and gaseous phases just become identical. At this critical point the *critical compressibility factor* Z_c is

$$Z_c = \frac{P_c V_c}{RT_c}$$

Since pressure, volume, and temperature are related to the corresponding critical properties, the function connecting the reduced properties becomes the same for each substance. The reduced property is expressed as a fraction of the critical property.

$$P_r = \frac{P}{P_c} \quad V_r = \frac{V}{V_c} \quad T_r = \frac{T}{T_c}$$

TABLE 5.3 Critical Properties

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Acetaldehyde	461	55	154
Acetic acid	594.4	57.1	171.3
Acetic anydride	569	46.2	290
Acetone	508.1	46.4	209
Acetonitrile	548	47.7	173
Acetophenone	701	38	376
Acetyl chloride	508	58	204
Acetylene	308.3	60.6	113
Acrylic acid	615	56	210
Acrylonitrile	536	45	210
Air	132.5	37.2	92.7
Allene	393		
Allyl alcohol	545	56.4	203
Allyl sulfide	653		
Aluminum trichloride	629	26	261
Aminoethanol	614	44	196
Ammonia	405.6	111.3	72.5
Aniline	699	52.4	270
Anisole	368	41.2	
Anthracene	883		
Antimony tribromide	904.5	56	
Antimony trichloride	794		270

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Argon	150.8	48.1	74.9
Arsine	373.0		
Benzaldehyde	695	46	
Benzene	562.1	48.3	259
Benzoic acid	752	45	341
Benzonitrile	699.4	41.6	
Benzyl alcohol	677	46	334
Biphenyl	789	38	502
Bismuth tribromide	1219		301
Bismuth trichloride	1179	118	261
Boron pentafluoride	470		
Boron tribromide	573		280
Boron trichloride	451.9	38.2	
Boron trifluoride	260.8	49.2	
Bromine	584	102	127
Bromobenzene	670	44.6	324
Bromoethane	503.8	61.5	215
Bromomethane	464	85	
Bromopentafluorobenzene	670	44.6	
Bromotrifluoromethane	340.2	39.2	200
1.2-Butadiene	443.7	44.4	219
1.3-Butadiene	425	42.7	221
Butane	425.2	37.5	255
1-Butanol	562.9	43.6	274
2-Butanol	536.0	41.4	268
2-Butanone	535.5	41.0	267
1-Butene	419.6	39.7	240
cis-2-Butene	435.6	41.5	234
trans-2-Butene	428.6	40.5	238
3-Butenenitrile	585	39	265
1-Buten-3-yne	455	49	202
Butyl acetate	579	31	400
1-Butylamine	524	41	288
<i>N</i> -Butylaniline	72	28	518
Butylbenzene	660.5	28.5	497
sec-Butylbenzene	664	29.1	
tert-Butylbenzene	660	29.3	
Butyl benzoate	723	26	561
Butylcyclohexane	667	31.1	
sec-Butylcyclohexane	669	26.4	
tert-Butylcyclohexane	659	26.3	
Butyl ethyl ether	531	30	390
1-Butyne	463.7	46.5	220
2-Butyne	488.6	502	221
Butyraldehyde	524	40	278
Butyric acid	628	52.0	292
Butyronitrile	582.2	37.4	285
Carbon dioxide	304.2	72.8	94.0
Carbon disulfide	552	78.0	170
Car John distillide	332	70.0	170

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Carbon monoxide	132.9	34.5	93.1
Carbon tetrachloride	556.4	45.0	276
Carbon tetrafluoride	227.6	36.9	140
Carbonyl chloride (phosgene)	455	56	190
Carbonyl sulfide	375	58	140
Chlorine	417	76.1	124
Chlorine pentafluoride	415.7	51.9	230.9
Chlorine trifluoride	426.6		
Chlorobenzene	632.4	44.6	308
1-Chlorobutane	542	36.4	312
2-Chlorobutane	520.6	39	305
1-Chloro-1, 1-difluoroethane	410.2	40.7	231
2-Chloro-1,l-difluoroethylene	400.5	44.0	197
Chlorodifluoromethane	369.2	49.1	165
Chloroethane	460.4	52.0	199
Chloroform	536.4	54.0	239
Chloromethane	416.3	65.9	139
2-Chloro-2-methylpropane	507	39	295
Chloropentafluoroacetone	410.7	28.4	
Chloropentafluoroethane	353.2	31.2	252
1-Chloropropane	503	45.2	254
2-Chloropropane	485	46.6	230
3-Chloropropene	514	47	234
Chlorotrifluoromethane	302.0	38.7	180
Chlorotrifluorosilane	308.5	34.2	
o-Cresol	697.6	49.4	282
m-Cresol	705.8	45.0	310
p-Cresol	704.6	50.8	277
Cyanogen	400	59	
Cyclobutane	459.9	49.2	210
Cycloheptane	589	36.7	390
Cyclohexane	553.4	40.2	308
Cyclohexanol	625	37	327
Cyclohexanone	629	38	312
Cyclohexene	560.4	42.9	292
Cyclopentane	511.6	44.5	260
Cyclopentanone	626	53	268
Cyclopentene	506.0		
Cyclopropane	397.8	54.2	170
Cymene	658		
cis-Decalin	702.2	31	
trans-Decalin	690.0	31	
Decane	617.6	20.8	603
Decanenitrile	621.9	32.1	
1-Decanol	700	22	600
1-Decene	615	21.8	650
Decylcyclohexane	750	13.4	
Decylcyclopentane	723.8	15.0	

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Deuterium			
(equilibrium)	38.3	16.28	60.4
(normal)	38.4	16.43	60.3
Deuterium bromide	361.9		
Deuterium chloride	328.4		
Deuterium hydride	35.8	14.64	62.8
Deuterium iodide	421.7		
Deuterium oxide	644.0	213.8	55.6
Diborane	289.0	39.5	
1,2-Dibromoethane	582.9	70.6	
Dibromomethane	583	71	
Dibromotetrafluoroethane	487.6	34	329
Dibutylamine	596	25	517
Dibutyl ether	580	25	500
1,2-Dichlorobenzene	697.3	40.5	360
1,3-Dichlorobenzene	684	38	359
1,4-Dichlorobenzene	685	39	372
Dichlorodifluoromethane	385.0	40.7	217
1,1-Dichloroethane	523	50	240
1,2-Dichloroethane	561	53	220
1,1-Dichloroethylene	544		
1,2-Dichloroethylene	516.5	54.4	
Dichlorofluoromethane	451.6	51.0	197
Dichloromethane	510	60.0	193
1,2-Dichloropropane	577	44	226
Dichlorosilane	449	46.1	220
1,1-Dichloro-1,2,2,2-tetrafluoroethane	418.6	32.6	294
1,2-Dichloro-1,1,2,2-tetrafluoroethane	418.9	32.6	293
Diethylamine	496.6	36.6	301
1,4-Diethylbenzene	657.9	27.7	480
Diethyl disulfide	642	27.7	100
Diethylene glycol	681	46	316
Diethyl ether	466.7	35.9	280
3,3-Diethylpentane	610	26.4	200
Diethyl sulfide	557	39.1	318
Difluoroamine (HNF ₂)	403	93	310
cis-Difluorodiazine (N_2F_2)	272	70	
trans-Difluorodiazine	260	55	
1.1-Difluoroethane	386.6	44.4	181
1,1-Difluoroethylene	302.8	44.0	154
Dihexyl ether	657	18	720
Dihydrogen disulfide	572	58.3	720
Dihydrogen distillide Dihydrogen heptasulfide	1015	33	
Dihydrogen hexasulfide	980	36	
Dihydrogen octasulfide Dihydrogen octasulfide	1040	30	
Dihydrogen pentasulfide	930	38.4	
Dihydrogen tetrasulfide Dihydrogen tetrasulfide	855	43.1	
Dihydrogen tetrasunide Dihydrogen trisulfide	738	50.6	
Diisopropyl ether	500	28.4	385
Dusopropyrenier	500	20.4	303

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
1,2-Dimethoxyethane	536	38.2	271
Dimethoxymethane	497		
Dimethylamine	437.6	52.4	187
<i>N</i> , <i>N</i> -Dimethylaniline	687	35.8	
2,2-Dimethylbutane	488.7	30.4	359
2,3-Dimethylbutane	499.9	30.9	358
2,3-Dimethyl-1-butene	501	32.0	343
2,3-Dimethyl-2-butene	524	33.2	351
3,3-Dimethyl-1-butene	490	32.1	340
1,1-Dimethylcyclohexane	591	29.3	416
cis-1,2-Dimethylcyclohexane	606	29.3	
<i>trans</i> -1,2-Dimethylcyclohexane	596	29.3	
cis-1,3-Dimethylcyclohexane	591	29.3	
trans-1,3-Dimethylcyclohexane	598	29.3	
1,1-Dimethylcyclopentane	547	34.0	360
cis-1,2-Dimethylcyclopentane	564.8	34.0	368
trans-1,2-Dimethylcyclopentane	553.2	34.0	362
Dimethyl ether	400.0	53.0	178
2,2-Dimethylhexane	549.8	25.0	478
2,3-Dimethylhexane	563.4	25.9	468
2,4-Dimethylhexane	553.5	25.2	472
2,5-Dimethylhexane	550.0	24.5	482
3,3-Dimethylhexane	562.0	26.2	443
3,4-Dimethylhexane	568.8	26.6	466
Dimethyl oxalate	628	39.2	400
2,2-Dimethylpentane	520.4	27.4	416
2,3-Dimethylpentane	537.3	28.7	393
2,4-Dimethylpentane	519.7	27.0	418
3,3-Dimethylpentane	536.3	29.1	414
2,2-Dimethylpropane	433.8	31.6	303
2,2-Dimethyl-1-propanol	549	39	319
2,3-Dimethylpyridine	655.4	37	317
2,4-Dimethylpyridine	644.2		
2,5-Dimethylpyridine	644		
2,6-Dimethylpyridine	623.7		
3,4-Dimethylpyridine	683.8		
3,5-Dimethylpyridine	667.2		
<i>N,N</i> -Dimethyl- <i>o</i> -toluidine	668	30.8	
1,4-Dioxane	587	51.4	238
Diphenyl ether	766	31.4	236
Diphenyl ether Diphenyl methane	767	29.4	
Dipropylamine	550	31	407
Dodecane	658.3	18.0	713
1-Dodecanol	679	19	713
1-Dodecanoi 1-Dodecene	657	18.3	/10
Dodecylcyclopentane	750	12.8	
Douecylcyclopeniane	/30	12.8	
Ethane	305.4	48.2	148
Ethanethiol	498.6	54.2	207
Luiancumui	770.0	J+.4	207

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Ethanol	516.2	63.0	167
Ethoxybenzene	647.1	33.8	
Ethyl acetate	523.2	37.8	286
Ethyl acetoacetate	673		
Ethyl acrylate	552	37.0	320
Ethylamine	456	55.5	178
Ethylbenzene	617.1	35.6	374
Ethyl benzoate	697	32	451
2-Ethyl-1-butanol	418.8		
Ethyl butyrate	565.9	30.2	395
Ethyl crotonate	599		
Ethylcyclohexane	609	29.9	450
Ethylcyclopentane	369.5	33.5	375
Ethylene	282.4	49.7	129
Ethylenediamine	592.9	62.1	206
Ethylene glycol	645	76	186
Ethylene oxide	469	71.0	140
Ethyl formate	508.4	46.8	229
3-Ethylhexane	565.4	25.7	455
2-Ethylhexanol	613	27.2	494
2-Ethyl-1-methylbenzene	651	30.0	460
3-Ethyl-1-methylbenzene	637	28.0	490
4-Ethyl-1-methylbenzene	640	29.0	470
Ethyl 3-methylbutyrate	588.0		
1-Ethyl-1-methylcyclopentane	592	29.5	
Ethyl methyl ether	437.8	43.4	221
Ethyl methyl ketone	535.6	41.0	267
3-Ethyl-2-methylpentane	567.0	26.7	443
3-Ethyl-2-methylpentane	576.5	27.7	455
3-Ethyl-3-methylpentane	576.4	27.7	455
Ethyl-2-methylpropanoate	553	30	410
Ethyl methyl sulfide	533	42	
3-Ethylpentane	540.6	28.5	416
o-Ethylphenol	703.0		
<i>m</i> -Ethylphenol	716.4		
<i>p</i> -Ethylphenol	716.4		
Ethylpropanoate	546.0	33.2	345
Ethyl propyl ether	500.6	32.1	244
o-Ethyltoluene	653	31	461
<i>m</i> -Ethyltoluene	636	31	461
<i>p</i> -Ethyltoluene	636	31	461
Ethyl vinyl ether	475	40.2	260
Fluorine	144.3	51.5	66.2
Fluorobenzene	560.1	44.9	271
Fluoroethane	375.3	49.6	169
Fluoromethane	317.8	58.0	124
Fluorotrichloromethane	471.1	43.2	248
Formaldehyde	408	65	

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Formic acid	580		
Furan	490.2	54.3	218
Germanium tetrachloride	550.0	38	330
Glycerol	726	66	255
Hafnium tetrabromide	746		415
Hafnium tetrachloride	723	57.0	304
Hafnium tetraiodide	916		528
Helium-3	3.30	1.167	73.2
Helium-4	5.19	2.24	57.3
Heptadecane	733	13	1000
1-Heptadecanol	736	14	
Heptane	540.2	27.0	432
1-Heptanol	633	30	435
1-Heptene	537.2	28	440
Heptylcyclopentane	679	19.2	
Hexadecane	717	14	
1-Hexadecene	717	13.2	
Hexadecylcyclopentane	791	9.6	
1,5-Hexadiene	507	34	328
Hexafluoroethane	292.8	29.4	223.7
Hexamethylbenzene	767		
Hexane	507.4	29.3	370
1-Hexanol	610	40	381
1-Hexene	504.3	31.3	350
cis-2-Hexene	518	32.4	351
trans-2-Hexene	516	32.3	351
cis-3-Hexene	517	32.4	350
trans-3-Hexene	519.9	32.1	350
Hexylcyclopentane	660.1	21.1	
Hydrazine	653	145	96.1
Hydrogen			
(equilibrium)	32.9	12.77	65.4
(normal)	33.2	12.8	65.0
Hydrogen bromide	363.2	84.4	100.0
Hydrogen chloride	324.6	82.0	81.0
Hydrogen cyanide	456.8	53.2	139
Hydrogen deuteride, see Deuterium hydride			
Hydrogen fluoride	461	64	69
Hydrogen iodide	424.0	82.0	131
Hydrogen selenide	411	88	
Hydrogen sulfide	373.2	88.2	98.5
Icosane	767	11.0	
1-Icosanol	770	12.0	
Iodine	819	115	155
Iodobenzene	721	44.6	351
Iodomethane	528	65	190

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Isobutyl acetate	561	30	414
Isobutylamine	516	42	284
Isobutylbenzene	650	31	480
Isobutyl butyrate	611		
lsobutylcyclohexane	659	30.8	
Isobutyl formate	551	38.3	350
Isobutyl 3-methylbutyrate	621		
Isobutyl propanoate	592		
Isobutyric acid	609	40	292
Isopropylamine	476	50	229
lsopropylbenzene	631.0	31.7	428
lsopropylcyclohexane	640	28	
Isopropylcyclopentane	601	29.6	
2-Isopropyl-1-methylbenzene	670	28.6	
3-Isopropyl-l-methylbenzene	666	290	
4-Isopropyl-1-methylbenzene	653	27.9	
Isoquinoline	803		
Isoxazole	552.0		
Ketene	380	64	145
Krypton	209.4	54.3	91.2
Mercury	1173	180	
Methane	190.6	45.4	99.0
Methanethiol	470.0	71.4	145
Methanol	512.6	79.9	118
Methoxybenzene (anisole)	641	41.2	
Methyl acetate	506.8	46.3	228
Methyl acrylate	536	42	265
Methylamine	430	73.6	140
N-Methylaniline	701	51.3	
Methyl benzoate	692	36	396
2-Methyl-1,3-butadiene	484	38.0	276
3-Methyl-1,2-butadiene	496	40.6	267
2-Methylbutane	460.4	33.3	306
2-Methyl-1-butanol	571	38	322
3-Methyl-1-butanol	579.5	38	329
2-Methyl-2-butanol	545	39	319
3-Methyl-2-butanone	553.4	38.0	310
2-Methyl-1-butene	465	34.0	294
2-Methyl-2-butene	470	34.0	318
3-Methyl-1-butene	450	34.7	300
Methyl butyrate	554.4	34.3	340
3-Methylbutyric acid	634		
Methylcyclohexane	572.1	34.3	368
Methylcyclopentane	532.7	37.4	319
N-Methylethylamine	496.6	36.6	243
Methyl formate	487.2	59.2	172
ivicuity i formate			

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
3-Methylheptane	563.6	25.1	464
4-Methylheptane	561.7	25.1	476
2-Methylhexane	530.3	27.0	421
3-Methylhexane	535.2	27.8	404
Methylhydrazine	567	79.3	271
Methyl isobutyrate	540.8	33.9	339
Methyl isocyanate	491	55	
1-Methylnaphthalene	772	35.2	445
2-Methylnaphthalene	761	34.6	462
2-Methylpentane	497.5	29.7	367
3-Methylpentane	504.4	30.8	367
2-Methyl-2,4-pentanediol	678	33.9	
4-Methyl-2-pentanone	571	32.3	371
2-Methyl-2-pentene	518	32.4	351
cis-3-Methyl-2-pentene	518	32.4	351
trans-3-Methyl-2-pentene	521	32.3	350
cis-4-Methyl-2-pentene	490	30	360
trans-4-Methyl-2-pentene	493	30	360
Methyl phenyl ether	641	41.2	300
2-Methylpropanal	513	41	274
2-Methylpropane	408.1	36.0	263
Methyl propanoate	530.6	39.5	282
2-Methyl-1-propanol (isobutyl alcohol)		42.4	273
2-Methyl-2-propanol			
* 1 1	506.2 417.9	39.2 39.5	275 239
2-Methylpropene		39.3	239
2-Methylpyridine	621		
3-Methylpyridine	645	4.4	211
4-Methylpyridine	646	44	311
α-Methylstyrene	654	33.6	397
Methyl vinyl ether	436	47	205
Morpholine	618	54	253
Naphthalene	748.4	40.0	410
Neon	44.4	27.2	41.7
Niobium pentabromide	1010		469
Niobium pentachloride	807		400
Niobium pentafluoride	737	62	155
Nitric oxide	180	64	58
Nitrobenzene	732		
Nitrogen-14	126.2	33.5	89.5
Nitrogen-15	126.3	33.5	90.4
Nitrogen dioxide (equilibrium)	431.4	100	170
Nitrogen trifluoride	234.0	44.7	
Nitromethane	588	62.3	173
Nitrosyl chloride	440	90	139
Nitrous oxide	309.6	71.5	97.4
Nitryl fluoride	349.4		
Nonadecane	756	11.0	
Nonane	594.6	22.8	548
1-Nonanol	677	I	546

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
1-Nonene	592	23.1	580
Nonylcyclopentane	710.5	16.3	
Octadecane	745	11.9	
1-Octadecanol	747	14	
1-Octadecene	739	11.2	
Octane	568.8	24.5	492
1-Octanol	658	34	490
2-Octanol	637	27	494
1-Octene	566.6	25.9	464
trans-2-Octene	580	27.3	
Octylcyclopentane	694	17.7	
Oxygen	154.6	49.8	73.4
Oxygen difluoride	215.2	48.9	97.7
Ozone	161.3	55.0	88.9
ozone -	101.5	22.0	00.5
Paraldehyde	563		
Pentachloroethane	646.1		
Pentadecane	707	15	880
1-Pentadecene	704	14.4	
Pentadecylcyclopentane	780	10.1	
1,2-Pentadiene	503	40.2	276
trans-1,3-Pentadiene	496	39.4	275
1.4-Pentadiene	478	37.4	276
Pentafluorobenzene	532.0	34.7	
1,1,2 <i>H</i> -Pentafluoropropane	380.11	31.0	273
Pentanal	554	35	333
Pentane	469.6	33.3	304
Pentanoic acid	651	38	340
1-Pentanol	586	38	326
2-Pentanone	564.0	38.4	301
3-Pentanone	561.0	36.9	336
1-Pentene	464.7	40.0	300
cis-2-Pentene	476	36.0	300
trans-2-Pentene	475	36.1	300
Pentyl formate	576		
1-Pentyne	493.4	40	278
Perchloryl fluoride	368.4	53.0	161
Perfluoroacetone	357.3	28.0	
Perfluorobenzene	516.7	32.6	
Perfluorobutane	386.4	22.9	378
Perfluoro-(2-butyltetrahydrofuran)	500.3	15.9	588
Perfluorocyclobutane	388.4	27.41	260
Perfluorocyclohexane	457.2	24	
Perfluorocyclohexene	461.8		
Perfluorodecene	542.3	14.3	
Perfluoroethane	292.8	29.4	223.7
Perfluoroheptane	474.8	16.0	664
Perfluoroheptene	478.1		
Perfluorohexane	451.7	18.8	442

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Perfluorohexene	454.3		
Perfluoromethylcyclohexane	486.8	23	
Perfluoronaphthalene	673.1		
Perfluorononane	524.0	15.4	
Perfluorooctane	502	16.4	
Perfluoropentane	422	20.1	
Perfluoropropane	345.1	26.5	299
Phenanthrene	878		
Phenetole	647	33.8	
Phenol	694.2	60.5	229
Phosgene	455	56	190
Phosphine	324.4	64.5	
Phosphonium chloride	322.2	72.7	
Phosphorus bromide difluoride	386	, 2.,	
Phosphorus chloride difluoride	362.32	44.6	
Phosphorus dibromide fluoride	527	11.0	
Phosphorus dichloride fluoride	463.0	49.3	
Phosphorus pentachloride	645	15.5	
Phosphorus trichloride	563		260
Phosphorus trifluoride	271.2	42.7	200
Phosphoryl chloride difluoride	423.8	43.4	
Phosphoryl trichloride	602	13.1	
Phosphoryl trifluoride	346.5	41.8	
Phthalic anhydride	810	47	368
Piperidine	594.0	47	289
Propadiene	393	54.0	162
Propane	369.8	41.9	203
1,2-Propanediol	625	60	237
1,3-Propanediol	658	59	241
Propanoic acid	612	53.0	230
1-Propanol	536.7	51.0	218.5
2-Propanol	508.3	47.0	220
2-Propenal	506.5	51	220
Propionaldehyde	496	47	223
Propionitrile	564.4	41.3	230
Propyl acetate	549.4	23.9	345
Propylamine	497.0	46.8	233
Propylbenzene	638.3	31.6	440
Propylogenzene Propylogenzene	603	29.6	425
Propylcyclohexane	639	27.7	723
Propylene	365.0	45.6	181
Propylene oxide	482.2	48.6	186
Propyl formate	538.0	40.1	285
Propyl propanoate	578	40.1	203
Propyr propanoate 1-Propyne	402.4	55.5	164
1-Propyne Pyridine	620.0	55.6	254
•	639.6	56	254
Pyrrole Pyrrolidine	568.6	55.4	249
i yrronume	0.600	33.4	249

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Quinoline	794.4		
Radon	376.9	62	139
Rhenium(VII) oxide	942		334
Selenium	1766		
Silane	269.6	47.8	
Silicon chloride trifluoride	307.6	34.2	
Silicon tetrachloride	507	37	326
Silicon tetrafluoride	259.1	36.7	
Silicon trichlorofluoride	438.5	35.3	
Styrene	647	39.4	
Sulfur	1314		
Sulfur dioxide	430.8	77.8	122
Sulfur hexafluoride	318.7	37.1	198
Sulfur tetrafluoride	364.0		420
Sulfur trioxide	491.0	81	130
Tantalum pentabromide	974		461
Tantalum pentachloride	767		400
o-Terphenyl	891.0	38.5	769
<i>m</i> -Terphenyl	924.8	34.6	784
p-Terphenyl	926.0	32.8	779
1,1,2,2-Tetrachloro-1,2-difluoroethane	551	34	370
1,1,2,2-Tetrachloroethane	661.1 620	44	290
Tetrachloroethylene Tetradecane	694	16	830
1-Tetradecene	689	15.4	830
Tetradecylcyclopentane	772	11.1	
Tetrafluoroethylene	306.4	38.9	175
Tetrafluorohydrazine	309.4	37	175
Tetrahydrofuran	540.2	51.2	224
1,2,3,4-Tetrahydronaphthalene	719	34.7	22 .
Tetrahydrothiophene	631.9	J	
1,2,4,5-Tetramethylbenzene	675	29	480
2,2,3,3-Tetramethylbutane	567.8	28.3	461
2,2,3,3-Tetramethylhexane	623.1	24.8	
2,2,5,5-Tetramethylhexane	581.5	21.6	
2,2,3,3-Tetramethylpentane	607.6	27.0	
2,2,3,4-Tetramethylpentane	592.7	25.7	
2,2,4,4-Tetramethylpentane	574.7	24.5	
2,3,3,4-Tetramethylpentane	607.6	26.8	
2-Thiapropane	503.1	54.6	201
Thiophene	579.4	56.2	219
Thymol	698		
Tin(IV) chloride	591.8	37.0	351
Titanium tetrachloride	638	46	340
Toluene	591.7	40.6	316
o-Toluidine	694	37	343
<i>m</i> -Toludine	709	41	343
<i>p</i> -Toluidine	667		
Toluonitrile	723		

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Tributylamine	643	18	
1,1,2-Trichloroethane	602	41	294
Trichloroethylene	571	48.5	256
Trichlorofluoromethane	471.2	43.5	248
1,2,3-Trichloropropane	651	39	348
1,2,2-Trichloro-1,1,2-trifluoroethane	487.2	33.7	304
Tridecane	675.8	17.0	780
1-Tridecene	674	16.8	
Tridecylcyclopentane	761	11.9	
Triethanolamine	787.4	24.2	
Triethylamine	535	30	390
Trifluoroacetic acid	491.3	32.2	204
1,1,1-Trifluoroethane	346.2	37.1	221
Trifluoromethane	298.89	47.7	133.3
Trimethylamine	433.2	40.2	254
1,2,3-Trimethylbenzene	664.5	34.1	430
1,2,4-Trimethylbenzene	649.1	31.9	430
1,3,5-Trimethylbenzene	637.3	30.9	433
2,2,3-Trimethylbutane	531.1	29.2	398
2,2,3-Trimethyl-1-butene	533	28.6	400
Trimethylchlorosilane	497.7	31.6	100
1,1,2-Trimethylcyclopentane	579.5	29.0	
1,1,3-Trimethylcyclopentane	569.5	27.9	
cis, cis, trans-	507.5	27.5	
1,2, 4-Trimethylcyclopentane	579	28.4	
cis,trans,cis-	317	20.1	
1,2, 4-Trimethylcyclopentane	571	27.7	
3,3,5-Trimethylheptane	609.6	22.9	
2,2,3-Trimethylhexane	588	24.6	
2,2,4-Trimethylhexane	573.7	23.4	
2,2,5-Trimethylhexane	567.9	23.0	519
2,2,3-Trimethylpentane	563.4	26.9	436
2,2,4-Trimethylpentane	543.9	25.3	468
2,3,3-Trimethylpentane	573.5	27.8	455
2,3,4-Trimethylpentane	566.3	26.9	461
2,2,4-Trimethyl-1,3-pentanediol	671	25.6	364.6
2,2,4 11methy1 1,5 pentanetho1	0/1	25.0	304.0
1 <i>H</i> -Undecafluoropentane	443.9		
Undecane	638.8	19.4	660
1-Undecene	637	19.7	
Uranium hexafluoride	505.8	45.5	250
Vinyl acetate	525	43	265
Vinyl chloride	429.7	55.3	169
Vinyl fluoride	327.8	51.7	114
Vinyl formate	475	57	210
Water	647.3	217.6	56.0
Xenon	289.7	57.6	118
o-Xylene	630.2	36.8	369

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TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
<i>m</i> -Xylene	617.0	35.0	376
<i>p</i> -Xylene	616.2	347	379
2,3-Xylenol	722.6	48	470
2,4-Xylenol	707.6	43	509
2,5-Xylenol	723.0	48	470
2,6-Xylenol	700.9	42	509
3,4-Xylenol	729.8	49	552
3,5-Xylenol	715.6	36	611
Zirconium tetrabromide	805		415
Zirconium tetrachloride	778	56.9	319
Zirconium tetraiodide	960		528
Zirconium tetraiodide	960	1	528

Estimation of Critical Properties

When the critical properties are unavailable, they may be estimated employing structural contributions to estimate T_c , P_c , and V_c . Lydersen's critical-property increments* provide good estimates for T_c and P_c ; Vetere's group contributions† yield reasonable estimates for V_c . The units employed are kelvins, atmospheres, and cubic centimeters per mole. Typical errors in estimated values are less than 2% for T_c but may rise up to 5% for higher-molecular-weight (greater than 100) nonpolar materials; errors are uncertain for molecules with multifunctional polar groups. Errors for estimated values of P_c and V_c are about double those for T_c .

The relations are

$$T_c = T_b \left[0.567 + \sum \Delta_T - \left(\sum \Delta_T \right)^2 \right]^{-1}$$

$$P_c = M \left(0.34 + \sum \Delta \right)^{-2}$$

$$V_c = 33 + \left[\sum_i \left(M_i \Delta_\nu \right) \right]^{1.029}$$

where T_b is the normal boiling point and M is the molular weight. Group contributions are listed in Table 5.4.

TABLE 5.4 Group Contributions for the Estimation of Critical Properties

There are no increments for hydrogen. All bonds shown as free are connected with atoms other than hydrogen. Values in parentheses are based upon very few experimental values.

Group	Δ_T , K	Δ_P , atm	Δ_V , cm ³ ·mol ⁻¹
	Nonrin	g increments	
—СН ₃ , —СН ₂ —	0.020	0.227	3.360 (linear chain) 2.888 (side chain)

^{*} A. L. Lydersen, Univ. Wisconsin Coll. Eng., Eng. Exp. Stn, Rep 3, Madison, April 1955.

[†] A Vetere, cited in R. C. Reid, J. M. Prausnitz, and T. K Sherwood, *The Properties of Gases and Liquids*, 3d ed., McGraw-Hill, New York, 1977, p. 17.

TABLE 5.4 Group Contributions for the Estimation of Critical Properties (*continued*)

		indicate of critical frop	erres (communear)
Group	Δ_T , K	Δ_P , atm	$_{V}$, cm ³ ·mol ⁻¹
—CH	0.012	0.210	3.360 (linear chain) 2.888 (side chain)
	0.0	0.210	3.360 (linear chain) 2.888 (side chain)
= CH ₂ , $=$ CH	0.018	0.198	2.940
=C-	0.0	0.198	2.940
=C=	0.0	0.198	2.908
\equiv CH, \equiv C $-$	0.005	0.153	2.648
=CII, =C- -0-	0.003	0.155	1.075
>C=0	0.040	0.29	1.765
>NH	0.031	0.135	2.333
>N $-$	0.014	0.17	1.793
—s—	0.015	0.27	0.591
	Ring	increments	
—CH ₂ —	0.013	0.184	2.813
CH			
	0.012	0.192	2.813
<u>-</u> Ç-	(-0.007)	(0.154)	2.813
=CH, $=$ C, $=$ C=	0.011	0.154	2.538
-0-	(0.014)	(0.12)	0.790
>C=0	(0.033)	(0.2)	1.500
>NH	(0.024)	(0.09)	1.736
>N-	(0.007)	(0.13)	1.883
s	(0.008)	(0.24)	0.911
	Genera	l substituents	
—F	0.018	0.224	0.770
—Cl	0.017	0.320	1.237
—Br	0.010	(0.50)	0.899
—I	0.012	(0.83)	0.702
—ОН		()	
Alcohols	0.082	0.06	0.704
Phenols	0.031	(-0.02)	1.553
HC=O(aldehyde)	0.048	0.33	2.333
—СООН	0.085	(0.4)	1.652
—COO— (ester)	0.047	0.47	1.607
-NH ₂	0.031	0.095	2.184
-CN	(0.060)	(0.36)	2.784
	1 1		
-NO ₂	(0.055)	(0.42)	1.559
—SH	0.015	0.27	1.537
— <u>\$</u> i—	0.03	(0.54)	

SECTION 6 SPECTROSCOPY

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	ACTION	

For more than half a century, spectroscopy has been the key structural tool for organic chemistry and biochemistry. This remains the case today although the availability of enhanced methods of X-ray analysis has somewhat altered the balance in both disciplines. A vast array of specialized texts are available that survey spectroscopic techniques in general or individual methods in particular. It would be folly to try to duplicate those efforts here. A brief overview of the methods may prove helpful and serve as a reminder for the practitioner who consults this handbook.

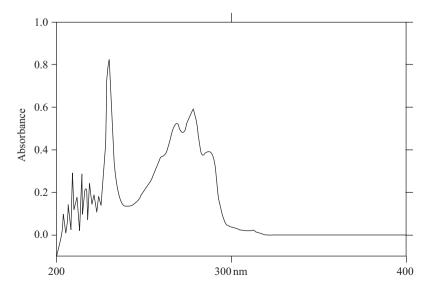
ULTRAVIOLET-VISIBLE SPECTROSCOPY

Generally, spectroscopic methods involve the absorption of radiation at certain wavelengths (and therefore certain energies) by molecules. For the techniques of ultraviolet–visible (UV–VIS) and infrared spectroscopy, there is an inverse proportionality between the amount of energy absorbed and the structural information that is revealed. The UV–VIS wavelength range is generally considered to be 200–800 nm. At the lower end, oxygen absorbs energy and the lowest end of the range is called the "vacuum UV." Relatively limited structural information may be obtained from the typically broad bands that are observed. Even so, the electronic transitions that are observed are sensitive to structure. Individual absorbing groups or chromophores absorb light at a characteristic wavelength. The absorption usually shifts when two or more chromophores are linked or in conjugation.

The UV-VIS technique may be used quantitatively by application of Beer's law:

$$\varepsilon = abc$$
.

In this relationship, ε is the extinction coefficient that is characteristic of a given compound. The values a and c represent absorption and concentration, respectively. The



UV Sprectrum of Napthalene.

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variable b is the pathlength of light through the sample, usually 1 cm. If the extinction coefficient is known, the measured absorption will give the compound's concentration.

The spectrum of naphthalene is shown above. Its broad bands reflect the absorption of energy by the extended pi-electron system.

The tables in this section present the essential data required for interpretation of UV–VIS spectra. Table 6.1 lists representative chromophores. These are identified by λ_{max} , the maximum height of any given peak, and by ε_{max} , the extinction coefficient at the maximum wavelength. Both the wavelength and absorption intensity are characteristic of individual chromophores.

Table 6.2 lists the ultraviolet cutoff for a variety of solvents commonly used in UV–VIS spectroscopy. The solvent chosen must dissolve the sample, yet be relatively transparent in the spectral region of interest. Typically, very low concentrations of sample will be present in the solvent. It is therefore important to avoid solvents that have even weak absorptions near the solute's bands of interest. Methanol and ethanol are two of the most commonly used solvents. Care must be exercised when using the latter that no benzene (an azeotropic drying agent) is present as this will alter the solvent's transparency. Normally, this will not be a problem in spectral grade solvents.

Tables 6.3–6.5 record data developed to undertake structural analysis in systems possessing chromophores that are conjugated or otherwise interact with each other. Chromophores within a molecule interact when linked directly to each other or when they are forced into proximity owing to structural constraints. Certain combinations of functional groups comprise chromophoric systems that exhibit characteristic absorption bands. In the era when UV–VIS was one of the principal spectral methods available to the organic chemist, sets of empirical rules were developed to extract as much information as possible from the spectra. The correlations referred to as Woodward's rules or the Woodward–Fieser rules, enable the absorption maxima of dienes (Table 6.3) and enones and dienones (Table 6.4) to be predicted. When this method is applied, wavelength increments correlated to structural features are added to the respective base values (absorption wavelength of parent compound). The data refer to spectra determined in methanol or ethanol. When other solvents are used, a numerical correction must be applied. These corrections are recorded in Table 6.5.

The benzene ring is a common structural element in organic chemistry. It is rigid and substituents are arranged in a fixed orientation. Shifts in the wavelength are expected for substituents that can interact electronically with the aromatic ring. Typically, shifts to longer wavelength (and intensification of the absorption band) are observed for any ring substitution. In the absence of conjugation, the shifts are small. Also, interposition of a single methylene group, or *meta* orientation within the aromatic ring, is sufficient to insulate chromophores almost completely from each other. With electron-withdrawing substituents, practically no change in the maximum position is observed. Directly conjugated groups may produce quite large spectral shifts. Examples include double and triple bonds and carbonyl groups. The spectra of heteroaromatics are related to their isocyclic analogs, but only in a general way. As with benzene, the magnitude of substituent shifts can be estimated, but tautomeric possibilities may invalidate the empirical method. Table 6.6 records data for substituents bonded directly to a benzene ring.

When electronically complementary groups are situated *para* to each other in disubstituted benzenes, there is a more pronounced shift to a longer wavelength than would be expected from the additive effect due to the extension of the chromophore from the electron-donating group through the ring to the electron-withdrawing group. When the *para* groups are not complementary, or when the groups are situated *ortho* or *meta* to each other, disubstituted benzenes show a more or less additive effect of the two substituents on the wavelength maximum. Calculation of the principal band of selected substituted benzenes is illustrated in Table 6.7.

TABLE 6.1 Electronic Absorption Bands for Representative Chromophores

Chromophore	System	$\lambda_{ m max}$	$oldsymbol{arepsilon}_{ ext{max}}$
Acetylene (ethynyl)	_C≡C—	175–180	6000
Aldehyde	—СНО	210	strong
		280-300	11–18
Amine	−NH ₂	195	2800
Azido	>C=N-	190	5000
Azo	_N=N-	285-400	3-25
Bromide	—Br	208	300
Carbonyl	>C=0	195	1000
		270-285	18-30
Carboxyl	—СООН	200-210	50-70
Disulfide	_s_s_	194	5 5 0 0
		255	400
Ester	—COOR	205	50
Ether	_o_	185	1000
Ethylene	-c=c-	190	8 000
Iodide	—I	260	400
Nitrate ester	-ONO ₂	270 (shoulder)	12
Nitrile	-C≡N	160	_
Nitrite ester	—ONO	220-230	1 000-2 000
		300-400	10
Nitro	-NO ₂	210	strong
Nitroso	-NO	302	100
Oxime	—NOH	190	5 000
Sulfone	—SO ₂ —	180	_
Sulfoxide	$>$ S=0($>$ S \rightarrow 0)	210	1 500
Thiocarbonyl	>c=s	205	strong
Thioether	_s_	194	4600
		215	1600
Thiol	—SH	195	1400
	$-(C=C)_2$ (acyclic)	210-230	21 000
	$-(C=C)_{3}-$	260	35 000
	—(C=C) ₄ —	300	52 000
	—(C=C) ₅ —	330	118 000
	$-(C=C)_2$ (alicyclic)	230-260	3000-8000
	C=C−C≡C	219	6500
	C=C-C=N	220	23 000
	C=C-C=0	210-250	10000-20000
		300-350	weak
	C=C-NO,	229	9500
Benzene		184	46700
		204	6900
		255	170
Diphenyl		246	20 000
Naphthalene		222	112000
r		275	5600
		312	175
Anthracene		252	199 000
1 man accine		375	7900
Phenanthrene		251	66000
i incliantimente	1	201	00000

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TABLE 6.1 Electronic Absorption Bands for Representative Chromophores (continued)

Chromophore	System	$\lambda_{ m max}$	$oldsymbol{arepsilon}_{ ext{max}}$
Naphthacene		272	180 000
1		473	12500
Pentacene		310	300 000
		585	12000
Pyridine		174	80000
•		195	6000
		257	1700
Quinoline		227	37 000
		270	3600
		314	2750
Isoquinoline		218	80000
•		266	4000
		317	3 500

 TABLE 6.2
 Ultraviolet Cutoffs of Spectrograde Solvents

Absorbance of 1.00 in a 10.0 mm cell vs. distilled water

Solvent	Wavelength, nm	Solvent	Wavelength, nm	
Acetic acid	260	Hexadecane	200	
Acetone	330	Hexane	210	
Acetonitrile	190	Isobutyl alcohol	230	
Benzene	280	Methanol	210	
1-Butanol	210	2-Methoxyethanol	210	
2-Butanol	260	Methylcyclohexane	210	
Butyl acetate	254	Methylene chloride	235	
Carbon disulfide	380	Methyl ethyl ketone	330	
Carbon tetrachloride	265	Methyl isobutyl ketone	335	
1-Chlorobutane	220	2-Methyl-1-propanol	230	
Chloroform (stabilized		N-Methylpyrrolidone	285	
with ethanol)	245	Nitromethane	380	
Cyclohexane	210	Pentane	210	
1,2-Dichloroethane	226	Pentyl acetate	212	
Diethyl ether	218	1-Propanol	210	
1,2-Dimethoxyethane	240	2-Propanol	210	
N,N-Dimethylacetamide	268	Pyridine	330	
N,N-Dimethylformamide	270	Tetrachloroethylene		
Dimethylsulfoxide	265	(stabilized with thymol)	290	
1,4-Dioxane	215	Tetrahydrofuran	220	
Ethanol	210	Toluene	286	
2-Ethoxyethanol	210	1,1,2-Trichloro-1,2,2-		
Ethyl acetate	255	trifluoroethane	231	
Ethylene chloride	228	2,2,4-Trimethylpentane	215	
Glycerol	207	o-Xylene	290	
Heptane	197	Water	191	

TABLE 6.3 Absorption Wavelength of Dienes

Heteroannular and acyclic dienes usually display molar absorptivities in the 8 000–20 000 range, whereas homoannular dienes are in the 5 000–8 000 range.

Poor correlations are obtained for cross-conjugated polyene systems such as

The correlations presented here are sometimes referred to as Woodward's rules or the Woodward-Fieser rules.

Base value for heteroannular or open chain diene, nm	214
Base value for homoannular diene, nm	253
Increment (in nm) for	
double bond extending conjugation	30
Alkyl substituent or ring residue	5
Exocyclic double bond	5
Polar groupings:	
-O-acyl	0
-O-alkyl	6
-S-alkyl	30
-Cl, -Br	5
-N (alkyl) ₂	60
Solvent correction (see Table 6.5)	
Calculated waveleng	th = total

TABLE 6.4 Absorption Wavelength of Enones and Dienones

$$o = c - \stackrel{\alpha}{c} = \stackrel{\beta}{c} \qquad o = c - \stackrel{\alpha}{c} = \stackrel{\beta}{c} - \stackrel{\gamma}{c} = \stackrel{\beta}{c} \stackrel{\gamma}{\rho}$$

Base values, nm	
Acyclic α,β -unsaturated ketones	215
Acyclic α, β -unsaturated aldehyde	210
Six-membered cyclic α,β -unsaturated ketones	215
Five-membered cyclic α , β -unsaturated ketones	214
α,β -Unsaturated carboxylic acids and esters	195
Increments (in nm) for	
Double bond extending conjugation:	
Heteroannular	30
Homoannular	69
Alkyl group or ring residue:	
lpha	10
β	12
γ,δ	18

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TABLE 6.4 Absorption Wavelength of Enones and Dienones (*continued*)

Polar groups:	
—OH	
α	35
$oldsymbol{eta}$	30
γ	50
$-$ O $-$ CO $-$ CH ₃ and $-$ O $-$ CO $-$ C ₆ H ₅ : $\alpha, \beta, \gamma, \delta$	8
—OCH ₃	
α	35
$oldsymbol{eta}$	30
	17
$rac{\gamma}{\delta}$	31
$-S$ —alkyl, β	85
—Cl	
α	15
β	12
—Br	
α	25
$oldsymbol{eta}$	30
$-N(alkyl)_2, \beta$	95
Exocyclic double bond	5
Solvent correction (see Table 6.5)	
	Calculated wavelength = total

TABLE 6.5 Solvent Correction for UV–VIS spectroscopy

Solvent	Correction, nm		
Chloroform	+1		
Diethyl ether	+11		
1,4-Dioxane	+5		
Ethanol	0		
Hexane	+11		
Methanol	0		
Water	-8		

 TABLE 6.6
 Primary Band of Substituted Benzene and Heteroaromatics

In methanol

Base value: 203.5 nm

Substituent	Wavelength shift, nm	Substituent	Wavelength shift, nm
—CH ₃	3.0	—СООН	25.5
$-CH=CH_2$	44.5	—COO-	20.5
—C≡CH	44	—CN	20.5
$-C_6H_5$	48	$-NH_2$	26.5
—F	0	$-NH_3^+$	-0.5
—Cl	6.0	$-N(CH_3)_2$	47.0
—Br	6.5	-NH-CO-CH ₃	38.5
—I	3.5	$-NO_2$	57
—OH	7.0	—SH	32
-0^{-}	31.5	$-SO-C_6H_5$	28
−OCH ₃	13.5	-SO ₂ CH ₃	13
$-OC_6H_5$	51.5	$-SO_2NH_2$	14.0
—СНО	46.0	$-CH=CH-C_6H_5$	
—CO—CH ₃	42.0	cis(Z)	79
$-CO-C_6H_5$	48	trans(E)	92.0
		—CH=CH—COOH, trans	69.5
	Base value,		Base value,
Heteroaromatic	nm	Heteroaromatic	nm
Furan	200	Pyridine	257
Pyrazine	257	Pyrimidine	ca 235
Pyrazole	214	Pyrrole	209
Pyridazine	ca 240	Thiophene	231

TABLE 6.7 Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives *In ethanol*

Base value of parent chromophore, nm		
C ₆ H ₅ COOH or C ₆ H ₅ COO—alkyl	230	
C_6H_5 —CO—alkyl (or aryl)	246	
C ₆ H ₅ CHO	250	
Increment (in nm) for each substituent on phenyl ring		
—Alkyl or ring residue		
o-, m-	3	
p-	10	
—OH and —O— alkyl		
o-, m-	7	
p-	25	
-0-		
0-	11	
m-	20	
p-	78*	

^{*} Value may be decreased markedly by steric hindrance to coplanarity.

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TABLE 6.7 Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives (continued)

—C1		
o-, m-	0	
p-	10	
—Br		
o-, m-	2	
p-	15	
$-NH_2$		
o-, m-	13	
p-	58	
-NHCO-CH ₃		
o-, m-	20	
<i>p</i> -	45	
-NHCH ₃		
<i>p</i> -	73	
$-N(CH_3)_2$		
o-, m-	20	
p-	85	
P	0.5	

PHOTOLUMINESCENCE

Luminescence processes may be categorized by the excitation method used with any particular luminescent molecule. Photoluminescence is the excitation process that involves the interaction of electromagnetic radiation with photons. The process is termed chemiluminescence when the exciting energy results from a chemical reaction. Any luminescence arising from an organism is referred to as bioluminescence.

The most common application of photoluminescence is found in fluorescence spectroscopy. Fluorescence is the immediate release of electromagnetic energy from an excited molecule or release of the energy from the singlet state. If the emitted energy arises from the triplet state or is delayed, the process is referred to as phosphorescence.

A fluorescence spectrum is characteristic of a given compound. It is observed as a result of radiative emission of the energy absorbed by the molecule. The observed spectrum does not depend on the wavelength of the exciting light, except that the spectrum will be more intense if irradiation occurs at the absorption maximum. The spectral intensity is called the quantum efficiency and is usually abbreviated as Φ . The quantum yield or quantum efficiency, Φ , which is solvent dependent, is the ratio: Φ = number of quanta emitted/number of quanta absorbed. Approximate values of quantum efficiencies are as follows: naphthalene, ~0.1; anthracene, ~0.3; indole, ~0.5; and fluorescein, ~0.9.

An equation similar to Beer's law applies to fluorescence spectroscopy at dilute concentrations. In its most general form, it is given as

$$F = \Phi I_o (1 - e^{-\varepsilon bc}).$$

In this equation, F is the observed fluorescence, Φ is the quantum efficiency (see above), I_0 is the intensity of the incident radiation, ε is the molar absorptivity, b is the cell's path length, and c is the compound's molar concentration.

The appearance of a fluorescence spectrum is reminiscent of a UV-VIS spectrum. The fluorescence spectrum for a 3-substituted indole derivative is shown in Figure 6.1. The

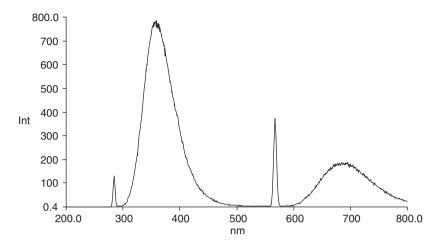


FIGURE 6.1 Fluorescence Spectrum for a 3-substituted indole derivative.

compound concentration was approximately $10^{-5}\,M$ in acetonitrile (CH₃CN). The sample was irradiated at a wavelength of 283 nm. The abscissa shows the wavelength in nanometers (nm) and the intensity ("int") is recorded on the ordinate. The maximum emission intensity is observed at 356 nm. The longest wavelength peak (λ_{max}) is observed at approximately 680 nm.

 TABLE 6.8
 Fluorescence Spectroscopy Data for Selected Organic Compounds

Compound	Solvent	pН	Excitation wavelength, nm	Emission wavelength, nm
Acenaphthene	Pentane		291	341
Acridine	CF₃COOH		358	475
Adenine	Water	1	280	375
Adenosine NH12 NOH OH	Water	1	285	395
Adenosine triphosphate	Water	1	285	395
Adrenalin			295	335
p-Aminobenzoic acid	Water	8	295	345

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 TABLE 6.8
 Fluorescence Spectroscopy Data for Selected Organic Compounds (continued)

	1			
Compound	Solvent	рН	Excitation wavelength, nm	Emission wavelength, nm
Aminopterin	Water	7	280, 370	460
II N NIII N NIII NIII NIII NIII NIII N				
1-Aminopyrene	CF₃COOH		330, 342	415
p-Aminosalicylic acid	Water	11	300	405
Amobarbital	Water	14	265	410
Anilines (aminobenzenes)	Water	7	280, 291	344, 361
Anthracene	Pentane		420	430
Anthranilic acid (2-aminobenzoic acid)	Water	7	300	405
Azaindoles	Water	10	290, 299	310, 347
Benz[c]acridine	CF₃COOH		295, 380	480
Benz[a]anthracene	Pentane		284	382
1,2-Benzanthracene			280, 340	390, 410
Benzanthrone	CF₃COOH		370, 420	550
Benzo[b]chrysene	Pentane		283	398
11-H-Benzo[a]fluorene	Pentane		317	340
Benzoic acid	70% H ₂ SO ₄		285	385
3,4-Benzopyrene (benzo[a]pyrene)	Benzene		365	390, 480
4,5-Benzopyrene (benzo[e]pyrene)	Pentane		329	389
Benzoquinoline	CF₃COOH		280	425
Benzoxanthane	Pentane		363	418
Bromolysergic acid diethylamide	Water	1	315	460
Brucine	Water	7	305	500
-	l .		1	1

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 TABLE 6.8
 Fluorescence Spectroscopy Data for Selected Organic Compounds (continued)

Compound	Solvent	pН	Excitation wavelength, nm	Emission wavelength, nm
Carbazole	N,N- Dimethyl- formamide		291	359
Carboxyfluorescein	Solvent		000	000
Chlortetracycline Chrysene	Pentane		355 250, 300, 310	445 260, 380
Cinchonine Coumarin	Water Ethanol	1	320 280	420 352
Dibenzo[a,c]anthracene	Pentane		280	381
Dibenzo[<i>b,k</i>]chrysene Dibenzo[<i>a,e</i>]pyrene 3,4,8,9-Dibenzopyrene	Pentane Pentane		308 370 370, 335,	428 401 480, 510
5,12-Dihydronaphthacene 1,4-Diphenylbutadiene Epinephrine Ethacridine Fluoranthrene	Pentane Pentane Water Water Pentane	7 2	390, 410 282 328 295 370, 425 354	340 370 335 515 464
Fluorene	Pentane		300	321

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 TABLE 6.8
 Fluorescence Spectroscopy Data for Selected Organic Compounds (continued)

Compound	Solvent	pН	Excitation wavelength, nm	Emission wavelength, nm
Fluorescein	Water	7–11	490	515
NH ₂				
COON				
HO O O O				
Folic acid	Water	7	365	450
Gentisic acid	Water	7	315	440
Griseofulvin	Water	7	295, 335	450
Guanine	Water	1	285	365
$H_{N} \xrightarrow{N} N \xrightarrow{N} H_{2N}$				
Harmine	Water	1	300, 365	400
$\underset{H_{3}CO}{\longleftarrow}\underset{H}{\stackrel{N}{\longleftarrow}}\underset{CH_{3}}{\stackrel{N}{\longleftarrow}}$				
Hippuric acid	70% H ₂ SO ₄		270	370
Homovanillic acid	Water	7	270	315
m-Hydroxybenzoic acid	Water	12	314	430
p-Hydroxycinnamic acid	Water	7	350	440
7-Hydroxycoumarin	Ethanol		325	441
5-Hydroxyindole	Water	1	290	355
5-Hydroxyindoleacetic acid	Water	7	300	355
3-Hydroxykynurenine	Water	11	365	460
p-Hydroxymandelic acid	Water	7	300	380
p-Hydroxyphenylacetic acid	Water	7	280	310
p-Hydroxyphenylpyruvic acid	Water	7	290	345
<i>p</i> -Hydroxyphenylserine	Water	1	290	320
5-Hydroxytryptophan	Water	7	295	340
Imipramine	Water	14	295	415
$\bigcap_{\substack{N\\ CH_2CH_2CH_2N(CH_3)_2}}$				
Indoleacetic acid	Water	8	285	360
Indoles	Water	7	269, 315	355
N _H				

6.15

 TABLE 6.8
 Fluorescence Spectroscopy Data for Selected Organic Compounds (continued)

Compound	Solvent	рН	Excitation wavelength, nm	Emission wavelength, nm	
-	***	-			
Indomethacin	Water	13	300	410	
Kynurenic acid	Water	7	325	405	
	***	11	325	440	
Lysergic acid diethylamide	Water	1	325	445	
Menadione	Ethanol		335	480	
9-Methylanthracene	Pentane		382	410	
3-Methylcholanthrene	Pentane		297	392	
7-Methyldibenzopyrene	Pentane		460	467	
2-Methylphenanthrene	Pentane		257	357	
3-Methylphenanthrene	Pentane		292	368	
1-Methylpyrene	Pentane		336	394	
4-Methylpyrene	Pentane		338	386	
Naphthacene (2,3-benzanthracene)			290, 310	480, 515	
1-Naphthol	0.1 M NaOH		365	480	
	20% ethanol				
2-Naphthol	0.1 M NaOH		356	426	
	20% ethanol				
Oxytetracycline			390	520	
Phenanthrene	Pentane		252	362	
Phenylalanine	Water		215, 260	282	
o-Phenylenepyrene	Pentane		360	506	
Phenylephrine			270	305	
Picene	Pentane		281	398	
Procaine	Water	11	275	345	
Pyrene	Pentane		330	382	
Pyridoxal	Water	12	310	365	
$H_{i,C}$ N OH					
Quinacrine	Water	11	285	420	
Quinidine	Water	1	350	450	
Quinine	Water	1	250, 350	450	

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TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (continued)

Compound	Solvent	pН	Excitation wavelength, nm	Emission wavelength, nm
Reserpine	Water	1	300	375
Resorcinol	Water		265	315
Riboflavin	Water	7	270, 370, 445	520
Rutin	Water	1	430	520
Salicylic acid	Water	11	310	435
Scoparone	Water	10	350, 365	430
Scopoletin	Water	10	365, 390	460
Serotonin	3 M HCl		295	550
Skatole	Water		290	370
Streptomycin	Water	13	366	445
<i>p</i> -Terphenyl	Pentane		284	338
Thiopental			315	530
Thymol	Water	7	265	300
Tocopherol	Hexane-		295	340
	ethanol			
Tribenzo[a,e,i]pyrene	Pentane		384	448
Triphenylene	Pentane		288	357
Tryptamine	Water	7	290	360
Tryptophan	Water	11	285	365
Tyramine	Water	1	275	310
Tyrosine	Water	7	275	310
Uric acid	Water	1 325		370
Vitamin A	1-Butanol	340		490
Vitamin B ₁₂	Water	7	275	305
Warfarin	Methanol		290, 342	385
Xanthine	Water	1	315	435
O N N N N N N N N N N N N N N N N N N N			275	305
3,4-Xylenol			280	310
Yohimbine	Water	1	270	360
Zoxazolamine	Water	11	280	320
Zoxazoiamine	water	11	280	320

TABLE 6.9 Fluorescence Quantum Yield Values

Compound	Solvent	Q_F value vs. Q_F standard		
	Q_F standard			
9-Aminoacridine	Water	0.99		
Anthracene	Ethanol	0.30		
POPOP*	Toluene	0.85		
Quinine sulfate dihydrate	1 N H ₂ SO ₄	0.55		
	Secondary standard	ls		
Acridine orange hydrochloride	Ethanol	0.54	Quinine sulfate	
		0.58	Anthracene	
1,8-ANS† (free acid)	Ethanol	0.38	Anthracene	
		0.39	POPOP	
1,8-ANS (magnesium salt)	Ethanol	0.29	Anthracene	
		0.31	POPOP	
Fluorescein	0.1 N NaOH	0.91	Quinine sulfate	
		0.94	POPOP	
Fluorescein, ethyl ester	0.1 N NaOH	0.99	Quinine sulfate	
		0.99	POPOP	
Rhodamine B	Ethanol	0.69	Quinine sulfate	
		0.70	Anthracene	
2,6-TNS‡ (potassium salt)	Ethanol	0.48	Anthracene	
		0.51	POPOP	

^{*} POPOP *p*-bis[2-(5-phenyloxazoyl)]benzene.

TABLE 6.10 Phosphorescence Spectroscopy of Some Organic Compounds

Abbreviation Used in the Table

EPA: diethyl ether, isopentane, and ethanol (5:5:2) volume ratio

Compound	Solvent	Lifetime,	Excitation wavelength, nm	Emission wavelength, nm
Acenaphthene	Ethanol		300	515
3-Acetylpyridine	Ethanol	0.5	395	525
Adenine	Water-methanol	2.9	278	406
	(9:1)			
Adenosine	Ethanol	0.8	280	422
p-Aminobenzoic acid	Ethanol		305	425
2-Aminofluorene	Ethanol	4.6	380	590
6-Amino-6-methylmercapto-	Water-methanol	0.66	321	456
purine	(9:1)			
2-Amino-4-methylpyrimidine	Ethanol	2.1	302	438

[†] ANS, anilino-8-naphthalenesulfonic acid.

[‡] TNS, 2-*p*-toluidinylnaphthalene-6-sulfonate.

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 TABLE 6.10
 Phosphorescence Spectroscopy of Some Organic Compounds (continued)

		Lifetime,	Excitation wavelength,	Emission wavelength,
Compound	Solvent	S	nm	nm
2-Amino-5-nitrobenzothiazole	EPA	0.41	375	515
2-Amino-5-nitrobiphenyl	EPA	0.56	380	520
3-L-Aminotyrosine · 2HCl	Ethanol	0.8	286	398
Anthracene	Ethanol		300	462
Aspirin	EPA	2.1	240	380
Atropine	Ethanol	1.4		410
8-Azaguanine	Ethanol	1.8	282	442
Benzaldehyde	Ethanol	3.4	254	433
1,2-Benzanthracene	Ethanol	2.2	310	510
Benzimidazole	Ethanol	2.3	280	406
Benzocaine	Ethanol	3.4	310	430
1,2-Benzofluorene	Ethanol		315	502
Benzoic acid	EPA	2.4	240	400
3,4-Benzopyrene	Ethanol		325	508
Benzyl alcohol	Ethanol		219	393
6-Benzylaminopurine	Water–methanol (9:1)	2.8	286	413
Biphenyl	Ethanol	1.0	270	385
6-Bromopurine	Water–methanol (9:1)	0.5	273	420
Brucine	Ethanol	0.9	305	435
Caffeine	Ethanol	2.0	285	440
Carbazole	Ethanol	7.8	341	436
2-Chloro-4-aminobenzoic acid	Ethanol	1.0	312	337
p-Chlorophenol	Ethanol	< 0.2	290	505
o-Chlorophenoxyacetic acid	Ethanol	0.7	280	518
<i>p</i> -Chlorophenoxyacetic acid	Ethanol	< 0.5	283	396
6-Chloropurine	Water–methanol (9:1)	0.64	273	419
Chlorpromazine · HCl	Ethanol	0.3	320	490
Chlorotetracycline	Ethanol	2.7	280	410
Cocaine · HCl	Ethanol	2.7	240	400
Codeine	Ethanol	0.3	270	505
Cytidine	Water–methanol (9:1)		290	420
Desoxypyridoxine · HCl	Ethanol	1.4	290	442
Diacetylsulfanilamide	Ethanol	1.3	280	405
2,6-Diaminopurine	Water–methanol	2.7	288	410
2,6-Diaminopurine sulfate	Ethanol	1.7	294	424
1,2,5,6-Dibenzanthracene	Ethanol	1.3	340	550
2,6-Dichloro-4-nitroaniline	EPA	0.5	368	525
2,4-Dichlorophenoxyacetic acid	Ethanol	< 0.5	289	490
2,6-Diethyl-4-nitroaniline	EPA	0.66	388	525
3,4-Dihydroxymandelic acid	Ethanol	1.1	294	412
3,4-Dihydroxyphenylacetic acid	Ethanol	0.9	295	430

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 TABLE 6.10
 Phosphorescence Spectroscopy of Some Organic Compounds (continued)

Compound	Solvent	Lifetime,	Excitation wavelength, nm	Emission wavelength, nm
2,5-Dimethoxy-4-methyl- amphetamine	Water–methanol (9:1)	3.9	289	411
5,7-Dimethyl-1,2-benzacridine	Ethanol	0.6	310	555
<i>N</i> , <i>N</i> -Dimethyl-4-nitroaniline	EPA	0.54	398	525
<i>N</i> , <i>N</i> -Dimethyltryptamine	Water-methanol (9:1)	6.9	286	434
Dopamine	Ethanol	0.9	285	430
Ephedrine	Ethanol	3.6	225	390
Epinephrine	Ethanol	1.0	283	425
N-Ethylcarbazole	Ethanol	7.8	340	437
Ethyl 3-indoleacetate	Ethanol	3.3	290	440
Folic acid	Ethanol		367	425
Hippuric acid	EPA	4.9	311	450
Homovanillic acid	Ethanol	0.8	289	435
DL-5-Hydroxytryptophan	Ethanol	6.3	315	435
Indole-3-acetic acid	Ethanol	< 0.5	290	438
3-Indoleacetonitrile	Ethanol	7.1	285	438
Indole-3-butonoic acid	Ethanol	0.6	284	510
Indolecarboxylic acid	Ethanol	5.5	290	429
Indole-2-propanoic acid	Ethanol	0.6	290	440
D-Lysergic acid	Water–methanol (9:1)	0.1	310	518
2-Methylcarbazole	Ethanol	8.1	333	442
N-Methylcarbazole	Ethanol	8.4	336	437
6-Methylmercaptopurine	Water–methanol (9:1)	0.6	291	420
N-Methyl-4-nitroaniline	EPA	0.5	390	522
6-Methylpurine	Water–methanol (9:1)	3.2	272	405
Morphine	Ethanol	0.3	285	500
Naphthacene	Ethanol		300	518
Naphthalene	EPA	1.8	310	475
1-Naphthaleneacetic acid	Ethanol	2.8	295	510
1-Naphthol	Ethanol	1.1	320	475
2-Naphthoxyacetic acid	Ethanol	2.6	328	497
2-Naphthylamine	Ethanol	2.3	270	303
Niacinamide	Ethanol		270	410
Nicotine	Ethanol	5.2	270	390
5-Nitroacenaphthene	EPA		380	540
4-Nitroaniline	EPA	0.6	380	510
9-Nitroanthracene	EPA		248	488
1-Nitroanthraquinone	EPA	0.3	250	490
4-Nitrobiphenyl	EPA		330	480
3-Nitro- <i>N</i> -ethylcarbazole	EPA	0.4	315	475
2-Nitrofluorene	EPA	0.4	340	517
6-Nitroindole	EPA	0.4	372	520
1-Nitronaphthalene	EPA		340	520

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 TABLE 6.10
 Phosphorescence Spectroscopy of Some Organic Compounds (continued)

Compound	Solvent	Lifetime,	Excitation wavelength, nm	Emission wavelength, nm
2-Nitronaphthalene	EPA	0.4	260	500
4-Nitro-1-naphthylamine	EPA		400	578
4-Nitrophenol	Ethanol	< 0.2	355	520
4-Nitrophenylhydrazine	EPA	0.5	390	520
4-Nitro-2-toluidine	EPA	0.5	375	520
Papaverine · HCl	Ethanal	1.5	260	480
Phenacetin	EPA			410
Phenanthrene	EPA	2.6	340	465
Phenobarbital	Ethanol	1.8	240	380
Phenylalanine	Ethanol		270	385
DL-2-Phenyllactic acid	Ethanol	5.4	262	383
Phthalylsulfathiazole	Ethanol	0.9	305	405
Procaine · HCl	Ethanol	3.5	310	430
Purine	Water–methanol (9:1)	2.2	272	405
Pyrene	Ethanol		330	515
Pyridine	Ethanol	1.4	310	440
Pyridine-3-sulfonic acid	Ethanol	1.2	272	408
Pyridoxine · HCl	Ethanol		290	425
Quercetin	Ethanol	2.1	345	480
Quinidine sulfate	Ethanol	1.3	340	500
Quinine · HCl	Ethanol	1.3	340	500
Salicyclic acid	Ethanol	6.2	315	430
Strychnine phosphate	Ethanol	1.2	290	440
Sulfabenzamide	Ethanol	0.7	305	405
Sulfadiazine	Ethanol	0.7	275	410
Sulfanilamide	Ethanol	2.9	300	410
Sulfapyridine	Ethanol	1.4	310	440
Sulfathiazole	Ethanol	0.9	310	420
1,2,4,5-Tetramethylbenzene	EPA	4.5	275	390
2-Thiouracil	Ethanol	< 0.5	310	430
2,4,5-Trichlorophenol	Ethanol	< 0.2	305	485
2,4,5-Trichlorophenoxyacetic acid	Ethanol	1.1	295	475
Triphenylene	Ethanol	15	290	460
Tryptophan	Ethanol	1.5	295	440
Tyrosine	Ethanol	2.8	290	390
Vitamin K ₁	Hexane	0.4	345	570
Vitamin K ₃	Hexane	0.5	335	510
Vitamin K ₅	Water–methanol (9:1)	1.3	310	535
Warfarin	Ethanol	0.8	305	460
Yohimbine · HCl	Ethanol	7.4	290	410

INFRARED SPECTROSCOPY

Infrared (IR) and Raman spectroscopy rely on the interaction of a bond between two elements and IR radiation in the 400–4000 cm⁻¹ range. The two techniques are distinct but closely related. Historically, infrared analysis has been the more widely used in organic chemistry but much of the brief discussion that follows applies equally to both methods.

A chemical bond may be considered as a spring to which two weights are attached. The weights are atoms of different atomic masses. The length and strength of the spring may be correlated to the length and strength of the chemical bond. Each bond will vibrate at a frequency that is characteristic of the attached atoms and the type of bond (*i.e.*, single, double, or triple) between them. Radiation of an appropriate frequency will be absorbed by the bond and the wavelength at which this occurs will be detected and recorded by the instrument in the spectrum. Indeed, most molecules have many bonds so multiple peaks are observed in an IR spectrum.

An electrical dipole is required for IR energy to be efficiently absorbed by a molecule. Thus, bonds between different elements will give more prominent absorption peaks than will symmetrical bonds. This is because the bond's dipole moment changes as the bond stretches and contracts. Symmetrical bonds do not change dipole moment even if the bond distance changes. Usually, the most prominent peaks are observed when the electronegativity difference between the bound elements is greatest. Thus, a C—O bond will usually be more prominent than a C—H bond.

The position (frequency) of the absorption depends on the strength of the bond linking them. Thus, single, double, and triple bonds are observed in characteristic ranges. In addition, the frequency is related to the masses of the attached atoms. The largest mass differences occur when an element is attached to hydrogen. Such bonds as C-H, O-H, and N-H typically are observed in the $2\,900-3\,600\,cm^{-1}$ range.

The remarkable versatility of NMR as an analytical method has diminished the importance of IR analysis in modern laboratories but it remains a very useful technique. The very small amount of sample required and the prominence of functional group absorption means that the progress of a reaction can be monitored very conveniently. For example, the reduction of an aldehyde to an alcohol will be accompanied by the disappearance of the prominent C=O peak and the appearance of a C—OH absorption. Because both peaks are so readily identifiable in a small sample, the reaction is easy to follow and its completeness can be assayed.

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen

	Abbreviatio m, moderately strong m-s, moderate to strong s, strong	ns Used in the Table var, of variable strength w, weak w-m, weak to moderately strong
Group	Band, cm ⁻¹	Remarks
	Sati	urated C—H
H -C-H H	2975–2950 (s) 2885–2865 (w)	Two or three bands usually; asymmetrical and symmetrical CH stretching, respectively. In

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm ⁻¹	Remarks
	Saturated C—H	I (continued)
		presence of double bond adjacent to CH ₃ group symmetrical band splits into two.
	1450–1260 (m)	Sensitive to adjacent negative substituents
	ca 2930 (s) 2870–2840 (w)	Frequency increased in strained systems. Symmetrical band splits
Н 		into two bands when double bond adjacent.
-C- acyclic	1480–1440 (m)	Scissoring mode
Н	ca 720 (w)	Rocking mode
	Alkane residues att	ached to carbon
Cyclopropane	ca 3050 (w)	CH stretching
	540–500 470–460 (s)	Aliphatic cyclopropanes
Cyclobutanes	580–490 (s)	Alkyl derivatives: 550–530 cm ⁻¹
Cyclopentanes	595–490 (s)	Alkyl derivatives: 585–530 cm ⁻¹
>C(CH ₃) ₂	ca 1380 (m)	A roughly symmetrical doublet
	1 175–1 165 (m) 1 150–1 130 (m)	If no H on central carbon, then one band at ca 1 190 cm ⁻¹
	1 130–1 130 (III)	one band at ca 1 190 cm
$-C(CH_3)_3$	1395–1385 (m)	Split into two bands
	1365 (s)	
Aryl-CH ₃	390–260 (m)	
Aryl-C ₂ H ₅	565–540 (m–s)	Toro handa
Aryl- C_3H_7 (or C_4H_9) —(CH_2) _n —	585–565 (m)	Two bands
n=1	785–770 (w-m)	Rocking vibrations
n=2	745–735 (w-m)	
n=3	735–725 (w–m)	
$n \ge 4$	725–720 (w–m)	
	Alkane residues attached t	o miscellaneous atoms
Epoxide C—H		
ŅН	ca 3 050 (m-s)	
>C—CH ₂	ca 3 050 (m-s)	
—CH ₂ —halogen	ca 3 050 (m-s)	Halogens except fluorine
	1435–1385 (m)	
	1300–1240 (s)	

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (continued)

Group	Band, cm ⁻¹	Remarks
Alkane	residues attached to miscella	aneous atoms (continued)
—СНО	2900–2800 (w) 2775–2700 (w) 1420–1370 (m)	
—CO—CH ₃	3 100–2 900 (w) 1 450–1 400 (s) 1 360–1 355 (s)	
—O—CH₃ ethers	2835–2810 (s) 1470–1430 (m–s) ca 1030 (w–m)	Two bands
—O—C(CH ₃) ₃	1200–1155 (s)	
OCH ₂ O	2790-2770 (m)	
—O—CH ₂ — esters	1475–1460 (m–s) 1470–1435 (m–s)	Acyclic esters. Frequency increased ca 30 cm ⁻¹ for cyclic and small ring systems.
—О—СО—СН ₃	1450-1400 (s) 1385-1365 (s) 1360-1355 (s)	Acetate esters The high intensity of these bands often dominates this region of the spectrum.
$-CH_2-\overset{ }{C}=C<$	1445-1430 (m)	
—CH ₂ —SO ₂ —	ca 1250 (m)	
P—CH ₃ Se—CH ₃ B—CH ₃	1320–1280 (s) ca 1280 (m) 1460–1405 (m) 1320–1280 (m)	
Si—CH ₃ Sn—CH ₃ Pb—CH ₃ As—CH ₃	1265–1250 (m–s) 1200–1180 (m) 1170–1155 (m) 1265–1240 (m)	
Ge—CH ₃ Sb—CH ₃ Bi—CH ₃ —CH ₂ —(Cd, Hg, Zn, Sn)	1240–1230 (m) 1215–1195 (m) 1165–1145 (m) 1430–1415 (m)	
N — CH_3 and N — CH_2 — N — CH_2 — CH_2 — N	2820–2780 (s) 1440–1390 (m) 1480–1450 (s)	Ethylenediamine complexes Ethylenediamine complexes

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm ⁻¹	Remarks		
Alk	Alkane residues attached to miscellaneous atoms (continued)			
N—CH ₃ Amine · HCl Amino acid · HCl Amides N—CH ₂ — amides	1 475–1 395 (m) 1 490–1 480 (m) 1 420–1 405 (s) ca 1 440 (m)			
S—CH ₃	2990–2955 (m–s) 2900–2865 (m–s) 1440–1415 (m) 1325–1290 (m) 1030–960 (m) 710–685 (w–m)			
S—CH ₂ —	2950–2930 (m) 2880–2845 (m) 1440–1415 (m) 1270–1220 (s)			
−С≡СН	ca 3 300 (s) 700–600	Sharp Bending		
C=C	3 040–3 010 (m)			
C=C H	3 095–3 075 (m) 2 985–2 970 (m)	CH stretching sometimes obscured by much stronger bands of saturated CH groups		
C=C H	995–980 (s) 940–900 (s) ca 635 (s) 485–445 (m–s)			
C=C H	895–885 (s) 560–530 (s) 470–435 (m)			
C = C	980–955 (s) 455–370 (m–s)			
C = C	730–655 (m) 670–455 (s)			
R H C=C R	850–790 (m) 570–515 (s) 525–470 (s)			

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm ⁻¹	Remarks
Alkane res	sidues attached to miscellan	eous atoms (continued)
-0-CH=CH ₂	965–960 (s) 945–940 (m) 820–810 (s)	
-S-CH=CH ₂	ca 965 (s) ca 860 (s)	
-CO-CH=CH ₂	995–980 (s) 965–955 (m)	
-CO-OCH=CH ₂	950–935 (s) 870–850 (s)	
-CO-C=CH ₂ -CO-OC=CH ₂ -O-CH=CH- trans -CO-CH=CH- trans	ca 930 (s) 880–865 940–920 (s) ca 990 (s)	
	Hydroxyl group O—H c	compounds
Primary aliphatic alcohols	3 640–3 630 (s) 1 350–1 260 (s)	Only in very dilute solutions in nonpolar solvents OH bending
Secondary aliphatic alcohols	1085-1030 (s) 3625-3620 (s)	Also broad band at 700–600 cm ⁻¹ See comments under primary aliphatic alcohols
	1350–1260 (s) 1125–1085 (s)	Also for α -unsaturated and cyclic tertiary aliphatic alcohols
Tertiary aliphatic alcohols	3620–3610 (s) 1410–1310 (s) 1205–1125 (s)	See comments under primary aliphatic alcohols
Aryl—OH	ca 3610 (s)	See comments under primary aliphatic alcohols
	1410–1310 (s) 1260–1180 (s) 1085–1030 (s)	Also for unsaturated secondary aliphatic alcohols
Carboxylic acids	3 300–2 500 (w–m) 995–915 (s)	Broad Broad diffuse band
Enol form of β -diketones	2700–2500 (var)	Broad

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm ⁻¹	Remarks
	Hydroxyl group O—H comp	ounds (continued)
Free oximes	3 600-3 570(w-m)	Shoulder
Free hydroperoxides	3560-3530 (m)	
Peroxy acids	ca 3 280 (m)	
Phosphorus acids	2700-2560 (m)	Broad
Water in solution	3710	When solution is damp
Intermolecular H bond Dimeric	3600–3500	Rather sharp. Absorptions arising from H bond with polar solvents also appear in this region.
Polymeric	3400-3200 (s)	Broad
Intramolecular H bond Polyvalent alcohols Chelation	3600–3500 (s) 3200–2500	Sharper than dimeric band above Broad and occasionally weak; the lower the frequency, the stronger the intramolecular bond
Water of crystallation (solid state spectra)	3600–3100 (w)	Usually a weak band at 1640– 1615 cm ⁻¹ also. Water in trace amounts in KBr disks shows a broad band at 3450 cm ⁻¹ .
	Amine, imine, ammonium, a	and amide N—H
Primary amines Aliphatic	3550-3300 (m) 1650-1560 (m) 1090-1020 (w-m)	Two bands in this range
	850–810 (w-m) 495–445 (m-s)	With α -carbon branching at 795 cm ⁻¹ and strong Broad
Aromatic	ca 290 (s) 1 350–1 260 (s) 445–345	Broad Also for secondary aryl amines
Amino acids	3100–3030 (m)	Values for solid states; broad bands also (but not always) near 2 500 and 200 cm ⁻¹
Amino salts	2800–2400 (m) 1625–1560 (m) 1550–1550 (m) 3550–3100 (m) ca 3380	Number of sharp bands; dilute solution Values for solid state Dilute solutions
	ca 3 280	2 Tate bolderons

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TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (continued)

Group	Band, cm ⁻¹	Remarks
	Amine, imine, ammonium, and a	amide N—H (continued)
Secondary amines	3550–3400 (w) 1580–1490 (w) 1190–1170 (m)	Only one band, whereas primary amines show two bands Often too weak to be noticed
Salts	1145–1130 (m) 455–405 (w–m) ca 2500 ca 2400 1620–1560 (m–s)	Sharp; broad values for solid state Sharp; broad values for solid state
Tertiary amines $R_1R_2R_3NH^+$	2700–2250	Group of relatively sharp bands; broad bands in solid state
Ammonium ion	3 300–3 030 (s) 1 430–1 390 (s)	Group of bands
Imines ==N=H	3350–3310 (w) 3490 (s) 3490 (s)	Aliphatic Aryl Pyrroles, indoles; band sharp
Imine salts	2700–2330 (m–s) 2200–1800 (m)	Dilute solutions One or more bands; useful to distinguish from protonated tertiary amines
Primary amide —CONH ₂	ca 3500 (m) ca 3400 (m)	Lowered ca 150 cm ⁻¹ in the solid state and on H bonding; often several bands 3 200–3 050 cm ⁻¹
Secondary amide — CONH—	3460-3400 (m) 3100-3070 (w)	Two bands; lowered on H bonding and in solid state. Only one band with lactams Extra band with bonded and solid-state samples
	Miscellaneous	R—Н
—S—H P—H O	2600–2550 (w) 2440–2350 (m) 2700–2560 (m) 100/137 times the	Weaker than OH and less affected by H bonding Sharp Associated OH
`OH R—D	corresponding RH frequency	Useful when assigning RH bands; deuteration leads to a known shift to lower frequency

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TABLE 6.12 Absorption Frequencies of Triple Bonds

Abbreviations Used in the Table

m, moderately strong m–s, moderate to strong var, of variable strength w-m, weak to moderately strong

s, strong

Aromatic

Cyanamides

Isonitriles $R - \stackrel{+}{N} \equiv \bar{C}$

>N-C \equiv N $\rightleftharpoons>$ $\stackrel{\scriptscriptstyle{\perp}}{N}-$ C= $\stackrel{\scriptscriptstyle{\perp}}{N}$

or R-N=C:

Band, cm⁻¹ Remarks Group Alkvnes Terminal 3300(s) CH stretching 2140-2100 (w-m)* C≡C stretching 1375-1225 (w-m) 695-575 (m-s) Two bands if molecule has axial symmetry ca 630 (s) Alkyl monosubstituted 2260-2150 (var)* Nonterminal Symmetrical or nearly symmetrical substitution makes the C≡C stretching frequency inactive. When more than one C≡C linkage is present, and sometimes when there is only one, there are frequently more absorption bands in this region than there are triple bonds to account for them. $R_1 - C \equiv C - R_2$ 540-465 (m) The longer the chain, the lower the frequency $Aryl-C \equiv C$ ca 550 (m) ca 350 (var) —C≡C—halogen (Cl, Br, I) 185–160 (var) Nitriles—C≡N Stronger and toward the lower end 2260–2200 (var) of the range when conjugated; occasionally very weak or absent Aliphatic 580-555 (m-s)

560–525 (m–s) 390–350 (s)

2175-2150 (s)

2150-2115 (s)

2225-2210 (s)

1595

Very sensitive to changes in

substituents

Not found for nitriles

580–540 (s) 430–380 (m)

^{*} Conjugation with olefinic or acetylenic groups lowers the frequency and raises the intensity. Conjugation with carbonyl groups usually has little effect on the position of absorption.

TABLE 6.12 Absorption Frequencies of Triple Bonds (*continued*)

Group	Band, cm ⁻¹	Remarks
Thiocyanates R—S—C≡N	2175–2140 (s)	Aryl thiocyanates at the upper end of the range, alkyl at the lower
	404–400 (s) ca 600 (m–s)	end Aliphatic derivatives
Nitrile <i>N</i> -oxides $-C \equiv N \rightarrow O$	2305–2285 (s) 1395–1365 (s)	Aryl derivatives
Diazonium salts R—N ⁺ ≡N	2300–2230 (m–s)	
Selenocyanates R—Se—C≡N	ca 2 160 (m-s) 545-520 ca 390 ca 350	

 TABLE 6.13
 Absorption Frequencies of Cumulated Double Bonds

Abbreviations Used in the Table

m–s, moderate to strong s, strong

vs, very strong w, weak

Group	Band, cm ⁻¹	Remarks
Carbon dioxide O=C=O	2349 (s)	Appears in many spectra as a result of inequalities in path length
Isocyanates —N=C=O	2275–2250 (vs)	Position unaffected by conjugation
Isoselenocyanates —N=C=Se	2 200–2 000 (s) 675–605	Broad; usually two bands
Azides $-N_3$ or $-N = \stackrel{+}{N} = \bar{N}$	2140-2030 (s) 1340-1180 (w)	Not observed for ionic azides
-N=C=N-	2155–2130 (s)	Split into unsymmetrical doublet by conjugation with aryl groups: 2145–2125 (vs) and 2115–2105 (vs)

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TABLE 6.13 Absorption Frequencies of Cumulated Double Bonds (*continued*)

Group	Band, cm ⁻¹	Remarks
Isothiocyanates —N=C=S	2140–1990 (vs) 649–600 (m–s) 565–510 (m–s) 470–440 (m–s)	Broad; usually a doublet
Ketenes >C=C=0	ca 2150 (s)	
Ketenimines C=C=N-	2050–2000 (s)	
Allenes >C=C=C	2000–1915 (m–s)	Two bands when terminal allene or when bonded to electron-attracting groups
Thionylamines —N=S=O	1300–1230 (s) 1180–1110 (s)	
Diazoalkanes $\begin{array}{c} R_2C = \stackrel{\uparrow}{N} = \bar{N} \\ -CH = \stackrel{\downarrow}{N} = \bar{N} \end{array}$	2030–2000 (s) 2050–2035 (s)	
Diazoketones —CO—CH—N —	2 100–2 080 2 075–2 050	Monosubstituted Disubstituted

Position of Carbonyl Absorption

Because the carbonyl absorption is one of the most prominent and identifiable bands in the IR spectrum, it is often used diagnostically. The general trends of structural variation on the position of C = O stretching frequencies are summarized in six principles, as follows. Details of carbonyl absorptions are recorded in Table 6.14 and for other double bonds in Table 6.15, for aromatic bonds in Table 6.16 and other miscellaneous bonds in Table 6.17.

- 1. The more electronegative the group X in the system R—CO—X—, the higher is the frequency.
- 2. α,β -Unsaturation lowers the frequency by 15–40 cm⁻¹, except in amides, where little shift is observed; if present it is usually to higher frequency.
- **3.** Further conjugation has relatively little effect.

- **4.** Ring strain in cyclic compounds causes a relatively large shift to higher frequency. This phenomenon provides a remarkably reliable test of ring size, distinguishing clearly between four-, five-, and larger-membered-ring ketones, lactones, and lactams. Six-membered-ring and larger ketones, lactones, and lactams show the normal frequency found for the open-chain compounds.
- 5. Hydrogen bonding to a carbonyl group causes a shift to lower frequency of 40–60 cm⁻¹. Acids, amides, enolized β-keto carbonyl systems, and *o*-hydroxyphenol and *o*-aminophenyl carbonyl compounds show this effect. All carbonyl compounds tend to give slightly lower values for the carbonyl stretching frequency in the solid state compared with the value for dilute solutions.
- **6.** Where more than one of the structural influences on a particular carbonyl group is operating, the net effect is usually close to additive.

An especially convenient aspect of IR spectroscopy is its practice. A small amount of sample can be pressed between two NaCl or KBr (Table 6.19) disks and the spectrum can be determined without further preparation. A spectrum so obtained is recorded as "neat" or "between salts." If the sample is a solid, it may be mixed in a mortar and pestle with KBr and then pressed into a disk. The salt disk may be placed directly in the IR beam. In neither case is there a concern about solvent peaks. Of course, solvents may be used. Carbon tetrachloride and chloroform are the most commonly used solvents when the compound requires dissolution. Alternately, the sample may be intimately mixed (mulled) with mineral oil (a hydrocarbon oil). The thick slurry may then be smeared on a salt disk and placed in the spectrometer. The brand of mineral oil used historically is Nujol and such slurries are still called "Nujol mulls." The transmission characteristics of potential solvents for IR spectroscopy may be found in Table 6.20.

Traditional analog spectrometers were calibrated by taking a second spectrum of polystyrene. The sharp 1641 cm⁻¹ band was recorded on the same sheet as the original spectrum. Modern Fourier transform instruments do not usually require this step but still require calibration.

TABLE 6.14 Absorption Frequencies of Carbonyl Bands

All bands quoted are strong.

Groups	Band, cm ⁻¹	Remarks
Acid anhydrides —CO—O—CO—		
Saturated	1 850–1 800 1 790–1 740	Two bands usually separated by about 60 cm ⁻¹ . The higher-frequency band is more intense in acyclic anhydrides, and the lower-frequency band is more intense in cyclic anhydrides.
Aryl and α,β -unsaturated	1 830–1 780 1 700–1 710	
Saturated five-ring	1 870–1 820 1 800–1 750	
All classes	1300-1050	One or two strong bands due to CO stretching

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TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm ⁻¹	Remarks
Acid chlorides—COCl		
Saturated	1815-1790	Acid fluorides higher, bromides and
Saturated	1015-1770	iodides lower
Aryl and α,β -unsaturated	1790–1750	
Acid peroxide		
CO-O-CO-		
Saturated	1820-1810	
	1800-1780	
Aryl and α,β -unsaturated	1805-1780	
	1785-1755	
Esters and lactones		
_co_o_		
Saturated	1750–1735	
Aryl and α, β -unsaturated	1730–1715	
Aryl and vinyl esters		
C=C-O-CO-alkyl	1800-1750	The C=C stretching band also
		shifts to higher frequency.
Esters with electronegative		
α substituents; e.g.,		
>CCl-CO-O-	1770-1745	
α-Keto esters	1755-1740	
Six-ring and larger lactones	Similar values to	
	the correspond-	
	ing open-chain	
	esters	
Five-ring lactone	1780–1760	
α,β -Unsaturated five-ring	1700 1700	
lactone	1770-1740	When α -CH is present, there are
idetolie	1770 1740	two bands, the relative intensity
		depending on the solvent.
β, γ -Unsaturated five-ring		depending on the sorvent.
lactone, vinyl ester type	ca 1 800	
Four-ring lactone	ca 1 820	
β -Keto ester in H bonding	ca 1 020	
enol form	ca 1 650	Voto from normal; abalata tuna
enoi ionn	ca 1 030	Keto from normal; chelate-type
		H bond causes shift to lower
		frequency than the normal ester.
		The C=C band is strong and is
	1200 1070	usually near 1630 cm ⁻¹ .
All classes	1300–1050	Usually two strong bands due to CO stretching
Aldehydes — CHO		Co stretching
(See also Table 6.39 for		
C—H.) All values given		
below are lowered in liquid-		
film or solid-state spectra by		
about 10–20 cm ⁻¹ . Vapor-		
about 10–20 cm · . vapor-		
phase spectra have values		
raised about 20 cm ⁻¹ .		

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm ⁻¹	Remarks
Aldahadaa CHO (aaadaaa A		
Aldehydes — CHO (continued)	1.7.40, 1.720	
Saturated	1740–1720	
Aryl	1715–1695	o-Hydroxy or amino groups shift this value to 1655–1625 cm ⁻¹ because of intramolecular H bonding.
α,β -Unsaturated	1705-1680	
$\alpha,\beta,\gamma,\delta$ -Unsaturated	1680-1660	
β -Ketoaldehyde in enol form	1670–1645	Lowering caused by chelate-type H bonding
Ketones >C=O All values given below are lowered in liquid-film or solid-state spectra by about 10–20 cm ⁻¹ . Vapor-phase spectra have values raised about 20 cm ⁻¹ .		
Saturated	1725-1705	
Aryl	1700-1680	
α , β -Unsaturated	1685-1665	
$\alpha,\beta,\alpha',\beta'$ -Unsaturated and diaryl	1670-1660	
Cyclopropyl	1705-1685	
Six-ring ketones and larger	Similar values to the correspond- ing open-chain ketones	
Five-ring ketones	1750–1740	α,β Unsaturation, $\alpha,\beta,\alpha',\beta'$ unsaturation, etc., have a similar effect on these values as on those of open-chain ketones.
Four-ring ketones	ca 1780	
α-Halo ketones	1745–1725	Affected by conformation; highest values are obtained when both
α, α' -Dihaloketones	1765–1745	halogens are in the same plane as the C=O.
1,2-Diketones, <i>syn-trans</i> -		
open chains	1730–1710	Anti-symmetrical stretching frequency of both C=O's. The symmetrical stretching is inactive in the infrared but active in the Raman.
syn-cis-1,2-Diketones, six-ring	1760 and 1730	
syn-cis-1,2-Diketones, five ring	1775 and 1760	
o-Amino-aryl or o-hydroxy-		
aryl ketones	1655–1635	Low because of intramolecular H bonding. Other substituents and steric hindrance affect the position of the band.

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TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm ⁻¹	Remarks
Ketones >C=O (<i>continued</i>)		
Quinones	1690–1660	C=C band is strong and is usually near 1 600 cm ⁻¹ .
Extended quinones	1655–1635	
Tropone	1650	Near 1 600 cm ⁻¹ when lowered by H bonding as in tropolones
Carboxylic acids — CO ₂ H		
All types	3000-2500	OH stretching; a characteristic group of small bands due to combination bands
Saturated	1725–1700	The monomer is near 1760 cm ⁻¹ , but is rarely observed. Occasionally both bands, the free monomer, and the H-bonded dimer can be seen in solution spectra. Ether solvents give one band near 1730 cm ⁻¹ .
α,β -Unsaturated	1715-1690	
Aryl	1700-1680	
lpha-Halo-	1740–1720	
Carboxylate ions — CO_2^-		
Most types	1610–1550	Anti-symmetrical and symmetrical
	1420-1300	stretching, respectively
Amides —CO—N<		
(See also Table 6.39 for		
NH stretching and bending.)		
Primary —CONH ₂ In solution	ca 1 690	And to C. Ontotalina
Solid state	ca 1 650	Amide I; C=O stretching
In solution	ca 1600	Amide II: mostly NH bending
Solid state	ca 1640	Aimac II. mostry WII bending
Solid state	Ca 1 040	Amide I is generally more intense
		than amide II. (In the solid state, amides I and II may overlap.)
Secondary —CONH—		T ,
In solution	1700-1670	Amide I
Solid state	1680-1630	
In solution	1550–1510	Amide II; found in open-chain amides only
Solid state	1570–1515	Amide I is generally more intense than amide II.
Tertiary	1670–1630	Since H bonding is absent, solid and solution spectra are much the same.
Lactams		
Six-ring and larger rings	ca 1 670	
Five-ring	ca 1700	Shifted to higher frequency when
Four-ring	ca 1745	the N atom is in a bridged system

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm ⁻¹	Remarks
R-CO-N-C=C		Shifted $+15 \mathrm{cm}^{-1}$ by the additional
		double bond
C=C-CO-N		Shifted by up to +15 cm ⁻¹ by the additional double bond. This is an unusual effect by α,β unsaturation. It is said to be due to the inductive effect of the C=C on the well-conjugated CO—N system, the usual conjugation effect being less
		important in such a system.
Imides —CO—N—CO—		
Cyclic six-ring	ca 1710 and	Shift of $+15 \mathrm{cm}^{-1}$ with α, β
	ca 1700	unsaturation
Cyclic five-ring	ca 1770 and ca 1700	
Ureas N—CO—N		
RNHCONHR	ca 1 660	
Six-ring	ca 1 640	
Five-ring	ca 1720	
Urethanes R—O—CO—N	1740–1690	Also shows amide II band when nonsubstituted on N
Thioesters and Acids RCO—S—R'		
RCOSH	ca 1720	α,β -Unsaturated or aryl acid or ester shifted about $-25 \mathrm{cm}^{-1}$
RCOS—alkyl	ca 1 690	25555 25555 2 40040 20011
RCOS—aryl	ca 1710	

TABLE 6.15 Absorption Frequencies of Other Double Bonds

Abbreviations Used in the Table

m, moderately strong vs, very strong m-s, moderate to strong w, weak var, of variable strength

Group	Band, cm ⁻¹	Remarks
	Alkenes >C=C<	
Nonconjugated Conjugated with aromatic ring	1 680–1 620 (w-m) 1 640–1 610 (m)	May be very weak if symmetrically substituted More intense than with unconjugated double bonds

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TABLE 6.15 Absorption Frequencies of Other Double Bonds

Al	kenes $>$ C $=$ C $<$ (co	ntinued)
Internal (ring)	3 060-2 995 (m)	Highest frequencies for smallest ring
Carbons: $n = 3$ n = 4 n = 5 $n \ge 6$	ca 1 665 (w-m) ca 1 565 (w-m) ca 1 610 (w-m) 1 370–1 340 (s) 1 650–1 645 (w-m)	Characteristic
Exocyclic C=C(CH ₂) _n $n = 2$ n = 3 $n \ge 4$	1780–1730 (m) ca 1680 (m) 1655–1650 (m)	
Fulvene	1645–1630 (m) 1370–1340 (s) 790–765 (s)	
Dienes, trienes, etc.	1650 (s) and 1600 (s)	Lower-frequency band usually more intense and may hide or overlap the higher-frequency band
α , β -Unsaturated carbonyl compounds	1640-1590 (m)	Usually much weaker than the C=O band
Enol esters, enol ethers, and enamies	1700-1650 (s)	
Imines	, oximes, and amidines	>C=N-
Imines and oximes Aliphatic α,β -Unsaturated and aromatic Conjugated cyclic systems	1690–1640 (w) 1650–1620 (m) 1660–1480 (var) 960–930 (s)	NO stretching of oximes
Imino ethers —O—C=N—	1 690–1 640 (var)	Usually a strong doublet
Imino thioethers —S—C=N=	1 640–1 605 (var)	
Imine oxides $> C = \dot{N} - \bar{O}$	1620-1550 (s)	
Amidines >N—C—N—	1 685–1 580 (var)	
Benzamidines Aryl—C=N=N	1630–1590	

TABLE 6.15 Absorption Frequencies of Other Double Bonds (continued)

Group	Band, cm ⁻¹	Remarks
Imines	, oximes, and amidines $>$ C=	=N— (continued)
Guanidine $>N-C=N N$	1725–1625 (s)	
Azines >C=N-N=C<	1 670–1 600	
Hydrazoketones —CO—C=N—N	1600–1530 (vs)	
	Azo compounds —N=	=N—
Azo — N — N — Aliphatic Aromatic cis (Z) trans (E)	ca 1575 (var) ca 1510 (w) 1440–1410 (w)	Very weak or inactive
Azoxy $-N^{\dagger}=N-$ Aliphatic 0° Aromatic	1590–1495 (m-s) 1345–1285 (m-s) 1480–1450 (m-s) 1340–1315 (m-s)	
$\overline{\text{Azothio} - N = \overset{\scriptscriptstyle{+}}{N} - \overset{\scriptscriptstyle{-}}{S} -}$	1 465–1 445 (w) 1 070–1 055 (w)	
	Nitro compounds N=	=0
Nitro C—NO ₂ Aliphatic Aromatic	ca 1560 (s) 1385–1350 (s) 1570–1485 (s)	The two bands are due to asymmetrical and symmetrical stretching of the N=O bond. Electron-withdrawing substituents adjacent to nitro group increase the frequency of the asymmetrical band and decrease that of the symmetrical frequency. See above remark; also bulky
	1380–1320 (s) 865–835 (s)	orthosubstituents shift band to higher frequencies. Strong H bonding shifts frequency to lower end of range. Strong and sometimes at ca 750 cm ⁻¹

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TABLE 6.15 Absorption Frequencies of Other Double Bonds

Group	Band, cm ⁻¹	Remarks
	Nitro compounds N=O (co	ontinued)
	580–520 (var)	
α , β -Unsaturated	1530–1510 (s)	
Nitroalkenes	1360–1335 (s)	
Nitrates — O — NO ₂	1650–1625 (vs)	
	1 285–1 275 (vs)	
	870–855 (vs)	
	760–755 (w-m)	
	710–695 (w-m)	
Nitramines >N—NO ₂	1630–1550 (s)	
_	1300-1250 (s)	
Nitrates —O—N=O	1680–1610 (vs)	Two bands
	815–750 (s)	Trans(E) form
	850–810 (s)	Cis(Z) form
	690–615 (s)	
Thionitrites—S—N=O	730–685 (m-s)	
Nitroso ≥C—N=O	1600–1500 (s)	
$N-\stackrel{\scriptscriptstyle{+}}{N}=\bar{O}$		
Aliphatic	1530-1495 (m-s)	
Aromatic	1 480–1 450 (m-s)	
	1 335–1 315 (m-s)	
Nitrogen oxides N→O		
Pyridine	1 320–1 230 (m-s)	
*	1 190–1 150 (m-s)	
Pyrazine	1380–1280 (m-s)	Affected by ring substituents
	1 040–990 (m-s)	
	ca 850 (m)	

TABLE 6.16 Absorption Frequencies of Aromatic Bands

Abbreviations Used in the Table

m, moderately strong

var, of variable strength m, moderately strong var, of variable strength w-m, weak to moderately strong

s, strong

Group	Band, cm ⁻¹	Remarks
Aromatic rings	ca 1 600 (m) ca 1 580 (m)	Stronger when ring is further
	ca 1 470 (m)	conjugated When substituent on ring is electron
	ca 1510 (m)	acceptor When substituent on ring is electron donor
Five adjacent H	900–860 (w-m)	
	770–730 (s) 720–680 (s)	
	625–605 (w-m)	
	ca 550 (w-m)	Substituents: $C = C$, $C = C$, $C = N$
1,2-Substitution	770–735 (s)	
1,2 Suestitution	555–495 (w-m)	
	470–415 (m-s)	
1,3-Substitution	810–750 (s)	
	560-505 (m)	
	460–415 (m-s)	490–460 cm ⁻¹ when substituents are
		electron-accepting groups
1,4-Substitution	860–800 (s)	
	650–615 (w-m)	520, 400, -1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1
	520–440 (m-s)	520–490 cm ⁻¹ when substituents are electron-donating groups
1,2,3-Trisubstitution	800–760 (s)	
	720–685 (s)	
	570–535 (s) ca 485	
1,2,4-Trisubstitution	900–885 (m)	
	780–760 (s)	
	475–425 (m-a)	
1,3,5-Trisubstitution	950–925 (var)	
	865–810 (s)	
	730–680 (m-s)	
	535–495 (s)	
	470–450 (w-m)	
Pentasubstitution	900–860 (m-s)	
	580–535 (s)	
Hexasubstitution	415–385 (m-s)	

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 TABLE 6.17
 Absorption Frequencies of Miscellaneous Bands

Abbreviations Used in the Table

m, moderately strong m-s, moderate to strong vs, very strong w, weak

s, strong

w-m, weak to moderately strong

var, of variable strength

Group	Band, cm ⁻¹	Remarks
	Ethers	
Saturated aliphatic ≥C−O−C€	1150–1060 (vs)	Two peaks may be observed for branched chain, usually 1 140–1110 cm ⁻¹ .
	1140–900 (s)	Usually 930–900 cm ⁻¹ ; may be absent for symmetric ethers
Alkyl-aryl	1270 1220 ()	60
=C-0-C€	1 270–1 230 (vs) 1 120–1 020 (s)	=CO stretching CO stretching
Vinyl	1225-1200 (s)	Usually about 1 205 cm ⁻¹
Diaryl		
=C-O-C=	1200–1120 (s) 1100–1050 (s)	
Cyclic	1270-1030 (s)	
Epoxides >C C<	1 260–1 240 (m-s) 880–805 (m) 950–860 (var) 865–785 (m) 770–750 (m)	Monosubstituted Trans (E) form Cis (Z) form Trisubstituted
Ketals and acetals	1190-1140 (s) 1195-1125 (s) 1100-1000 (s) 1060-1035 (s)	Strongest band Sometimes obscured
Phthalanes	915–895 (s)	
Aromatic methylenedioxy	1265–1235 (s)	
	Peroxides	I
-0-0-	900–830 (w) 1150–1030 (m-s) ca 1000 (m)	Alkyl Aryl

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks		
Sulfur compounds				
Thiols —S—H —CO—SH —CS—SH	2600–2450 (w) 840–830 (m) ca 860 (s)	Broad		
Thiocarbonyl >C=S >N-C=S -S-C=S	1 200–1 050 (s) 1 570–1 395 1 420–1 260 1 140–940 ca 580 (s)	Behaves generally in a manner similar to carbonyl band		
Sulfoxides >S=O	1075–1040 (vs) 730–690 (var) 395–360 (var)	Halogen or oxygen atom bonded to sulfur increases the frequency.		
Sulfones >SO ₂	1360–1290 (vs) 1170–1120 (vs) 610–545 (m-s) 525–495 (m-s)	Halogen or oxygen atom bonded to sulfur increases the frequency.		
Sulfonamides —SO₂—N<	1380–1330 (vs) 1170–1140 (vs) 950–860 (m) 715–700 (w-m)			
Sulfonates —SO ₂ —O—	1420–1330 (s) 1200–1145 (s)	May appear as doublet		
Thiosulfonates —SO ₂ —S—	ca 1 340 (vs)			
Sulfates —O—SO ₂ —O— Primary alkyl salts	1415–1380 (s) 1200–1185 (s) 1315–1220 (s) 1140–1075 (m)	Electronegative substituents increase frequencies. Strongly influenced by metal ion		

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TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks		
Sulfur compounds (continued)				
Sulfates —O—SO ₂ —O (continued) Secondary alkyl salts	1270–1210 (vs) 1075–1050 (s)	Doublet; both bands strongly influenced by metal ion		
Stretching frequencies of C—S and S—S bonds $-S-CH_3$ $-S-CH_2-$ $-S-CH \le -S-CH \le -S-$	710–685 (w-m) 660–630 (w-m) 630–600 (w-m) 600–570 (w-m) 1110–1070 (m) 710–685 (w-m) 705–570 (w) 520–500 (w) 500–430 (w-m) 695–655 (w-m) 880–825 (s) 570–560 (var) 1035–935 (s) ca 580 (s) 1050–900 (m-s) 980–850 (m-s)	CSC stretching Monoionic Ionic 1,1-dithiolates		
	Phosphorus compound	ds		
Р—Н	2455–2265 (m) 1150–965 (w-m)	Sharp. Phosphines lie in the region 2285–2265 cm ⁻¹ .		
—PH ₂	1 100–1 085 (m) 1 065–1 040 (w-m) 940–910 (m)			
P—alkyl	795–650 (m-s)			
P—aryl	1130–1090 (s) 750–680 (s)			
P—O—alkyl	1050–970 (s)	Broad		
P—O—aryl	1240–1190 (s)			
Р—О—Р	970–910	Broad		

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks
	Phosphorus compounds (con	ntinued)
P=O	1350-1150 (s)	May appear as doublet
O	2725–2520 (w-m) 2350–2080 (w-m)	H-bonded; broad Broad; may be doublet for aryl acids
ОН	1740–1600 (w-m) 1335 (s) 1090–910 (s) 540–450 (w-m)	P=O stretching
P=S	865–655 (m-s) 595–530 (var)	
SOH	3 100–3 000 (w) 2 360–2 200 (w) 9 35–9 10 (s) 8 10–7 50 (m-s) 6 55–5 85 (var)	PO stretching P=S stretching P=S stretching
	Silicon compounds	
Si—H	2 250–2 100 (s) 985–800	SiH ₃ has two bands.
Si−C€	860–760	Accompanied by CH ₂ rocking
Si—CH ₃	1 280–1 250 (s)	Sharp
Si—C ₂ H ₅	1 250-1 220 (m) 1 020-1 000 (m) 970-945 (m)	
Si — Aryl	1 125–1 090 (vs)	Splits into two bands when two aryl groups are attached to one silicon atom, but has only one band when three aryl groups attached
∋Si—OH	870–820	OH deformation band
⇒Si-O-Si€	1 100–1 000	
⇒Si−N−Si€	940–870 (s)	
⇒Si—Cl	550–470 (s) 250–150	

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TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks
	Silicon compounds (con	tinued)
>SiCl ₂ 595–535 (s) 540–460 (m)		
—SiCl ₃	625–570 (s) 535–450 (m)	
	Boron compounds	S
Boranes >BH or —BH ₂	2640–2450 (m-s) 2640–2570 (m-s)	Free H in BH Free H in BH $_2$ plus second band
	2535–2485 (m-s) 2380–2315 (s) 2285–2265 (s)	In complexes; second band for BH_2
	2 140–2 080 (w-m) 2 580–2 450 (m)	Bridged H Borazoles and borazines
BH ₄ ⁻	2310–2195 (s)	Two bands
B—N	1 550–1 330 750–635	Borazines and borazoles
В—О	1 390–1 310 (s) 1 280–1 200	BO stretching Metal orthoborates
B—Cl B—Br	1 090–890 (s)	Plus other bands at lower frequencies for BX_2 and BX_3
В—Г	1 500–840 (var)	Isotope splitting present
XBF_2	1500–1410 (s) 1300–1200 (s)	
X_2BF	1 360–1 300 (s)	
BF ₃ complexes	1 260–1 125 (s) 1 030–800 (s)	Band splitting may be added to isotopic splittings.
BF ₄	ca 1 030 (vs)	

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TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (continued)

Group	Band, cm ⁻¹	Remarks
	Halogen compou	nds
C—F		
Aliphatic, mono-F Aliphatic, di-F	1110–1000 (vs) 780–680 (s) 1250–1050 (vs)	Two bands
Aliphatic, poly-F Aromatic	1360–1090 (vs) 1270–1100 (m) 680–520 (m-s) 420–375 (var) 340–240 (s)	Number of bands
—CF ₃		
Aliphatic	1350–1120 (vs) 780–680 (s) 680–590 (s) 600–540 (s)	
Aromatic	555–505 (s) 1330–1310 (m-s) 600–580 (s)	
C—Cl		
Primary alkanes	730–720 (s) 685–680 (s)	
Secondary alkanes	660–650 (s) ca 760 (m) 675–655 (m-s) 615–605 (s)	
Tertiary alkanes	635–610 (m-s) 580–560 (m-s)	
Poly-Cl Aryl:	800–700 (vs)	
1,2- 1,3-	1 060–1 035 (m) 1 080–1 075 (m)	
1,4-	1 100–1 090 (m)	
Chloroformates	ca 690 (s) 485–470 (s)	
Axial Cl Equatorial Cl	730–580 (s) 780–740 (s)	
C—Br Primary alkanes	645–635 (s) 565–555 (s)	
Secondary alkanes	440–430 (var) 620–605 (s) 590–575 (m-w) 540–530 (s)	

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TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks
	Halogen compounds (cont	tinued)
C—Br (continued)		
Tertiary alkanes	600–595 (m-s)	
•	525–505 (s)	
Axial	690–550 (s)	
Equatorial	750–685 (s)	
Aryl:		
1,2-	1 045-1 025 (m)	
1,3-; 1,4-	1 075-1 065 (m)	
Other bands	400–260 (s)	
	325–175 (m-s)	
	290–225 (m-s)	
C—I		
Primary alkanes	600–585 (s)	
•	515–500 (s)	
Secondary alkanes	ca 575 (s)	
•	550–520 (s)	
	490–480 (s)	
Tertiary alkanes	580–560 (s)	
	510-485 (m)	
	485–465 (s)	
Aromatic	1 060-1 055 (m-s)	
	310–160 (s)	
	265–185	
Axial	ca 640 (s)	
Equatorial	ca 655 (s)	
	Inorganic ions	
Ammonium	3 300–3 030	Several bands, all strong
-		Severar bands, an strong
Cyanate	2220–2130 (s)	
Cyanide	2200–2000	
Carbonate	1450–1410	
Hydrogen sulfate	1190-1160 (s)	
	1180-1000 (s)	
	880-840 (m)	
Nitrate	1410–1350 (vs)	
	860–800 (m)	
Nitrite	1275-1230 (s)	
	835–800 (m)	Shoulder

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm ⁻¹	Remarks
Inorganic ions (continued)		ued)
Phosphate	1 100–1 000	
Sulfate	1130-1080 (s)	
Thiocyanate	ca 2050 (s)	

 TABLE 6.18
 Absorption Frequencies in the Near Infrared

Values in parentheses are molar absorptivity

Class	Band, cm ⁻¹	Remarks
Acetylenes	9800–9430 6580–6400 (1.0)	Overtone of ≡CH stretching
Alcohols (nonhydrogen-bonded)	7140–7010 (2.0)	Overtone of OH stretching
Aldehydes		
Aliphatic	4640–4520 (0.5)	Combination of C=O and CH stretchings
Aromatic	ca 8 000 ca 4 525 ca 4 445	g.
Formate	4775–4630 (1.0)	
Alkanes		
—СН ₃	9 000–8 350 (0.02) 5 850–5 660 (0.1)	
—СН ₂ —	4510–4280 (0.3) 9170–8475 (0.02) 5830–6640 (0.1)	
≥CH	4420–4070 (0.25) 8550–8130 7000–6800	All bands very weak
Cyclopropane	5650–5560 6160–6060 4500–4400	
Alkenes		
C=C	6850–6370 (1.0)	
H >C=CH ₂ and -CH=CH ₂	7580–7300 (0.02) 6140–5980 (0.2) 4760–4700 (1.2)	

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TABLE 6.18 Absorption Frequencies in the Near Infrared (*continued*)

Class	Band, cm ⁻¹	Remarks
Alkenes (continued) H H	4760–4660 (0.15)	Trans (E) isomers have no unique bands.
C-C	6250-6040 (0.3)	
C=C	7580–7410 (0.02)	
,	6190–5990 (0.3)	
-0-CH=CH ₂	4820-4750	
$-CO-CH=CH_2$	(0.2–0.5)	
Amides		
Primary	7400–6540 (0.7)	Two bands; overtone of NH stretch
	5160-5060 (3.0)	Second overtone of C=O
	5040-4990 (0.5)	stretch; second overtone of
	4960–4880 (0.5)	NH deformation; combination of C=O and NH
Secondary	7330–7140 (0.5)	Overtone of NH stretch
	5050-4960 (0.4)	Combination of NH stretch and NH bending
Amines, aliphatic		
Primary	9710–9350	Second overtone of NH stretch
11111111	6670–6450 (0.5)	Two bands; overtone of NH
	5075-4900 (0.7)	Two bands; combination of NH stretch and NH bending
Secondary	9800-9350	Second overtone of NH stretch
y	6580–6410 (0.5)	Overtone of NH stretch
Amines, aromatic		
Primary	9950–9520 (0.4)	
	7 040–6 850 (0.2)	
	6760–6580 (1.4)	
	5 140–5 040 (1.5)	
Secondary	10000–9710	
	6800–6580 (0.5)	
Aryl-H	7660–7330 (0.1)	
	6170–5880 (0.1)	Overtone of CH stretch
Carbonyl	5 200–5 100	
Carboxylic acids	7000–6800	
Epoxide (terminal)	6135–5960 (0.2)	
	4665–4520 (1.2)	Cyclopropane bands in same region

TABLE 6.18 Absorption Frequencies in the Near Infrared (*continued*)

Class	Band, cm ⁻¹	Remarks
Glycols	7140–7040	
Hydroperoxides		
Aliphatic	6940-6750 (2.0)	
_	4960-4880 (0.8)	
Aromatic	7 040-6760 (1.0)	Two bands
	4950–4850 (1.3)	
Imides	9900–9620	
	6540–6370	
Nitriles	5 350-5 200 (0.1)	
Oximes	7140–7050	
Phosphines	5 350–5 260 (0.2)	
Phenols		
Nonbonded	7 140–6 800 (3.0)	
	5 000-4 950	
Intramolecularly bonded	7000–6700	
Thiols	5100-4950 (0.05)	

TABLE 6.19 Infrared Transmitting Materials

Material	Wavelength range, µm	Wavenumber range, cm ⁻¹	Refractive index at 2 µm
NaCl, rock salt	0.25–17	40000-590	1.52
KBr, potassium bromide	0.25-25	40 000-400	1.53
KCl, potassium chloride	0.30-20	33 000-500	1.5
AgCl, silver chloride*	0.40-23	25 000-435	2.0
AgBr, silver bromide*	0.50-35	20000-286	2.2
CaF ₂ , calcium fluoride (Irtran-3)	0.15–9	66 700-1 110	1.40
BaF ₂ , barium fluoride	0.20-11.5	50000-870	1.46
MgO, magnesium oxide (Irtran-5)	0.39-9.4	25 600-1 060	1.71
CsBr, cesium bromide	1–37	10 000-270	1.67
CsI, cesium iodide	1–50	10 000-200	1.74
TlBr-TlI, thallium bromide-iodide (KRS-5)*	0.50–35	20 000–286	2.37
ZnS, zinc sulfide (Irtran-2)	0.57-14.7	17 500–680	2.26

^{*} Useful for internal reflection work.

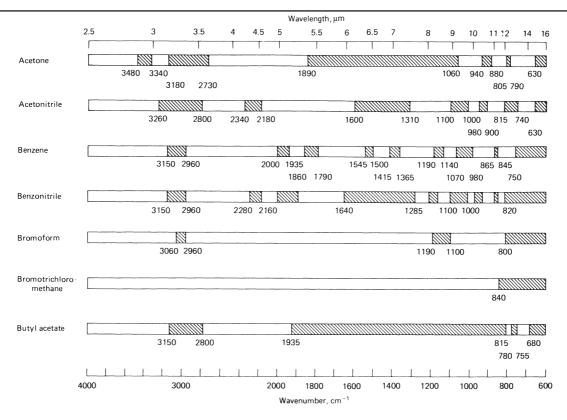
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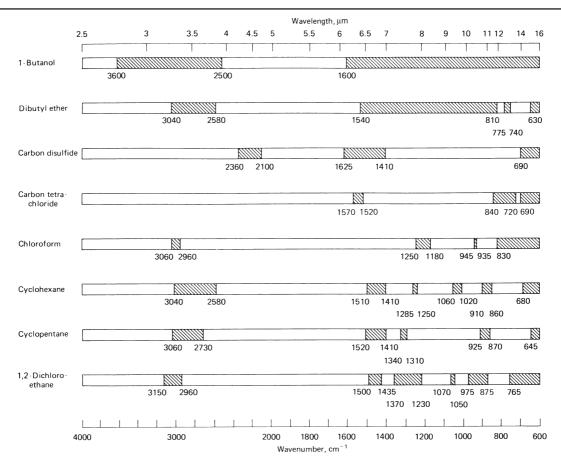
TABLE 6.19 Infrared Transmitting Materials (continued)

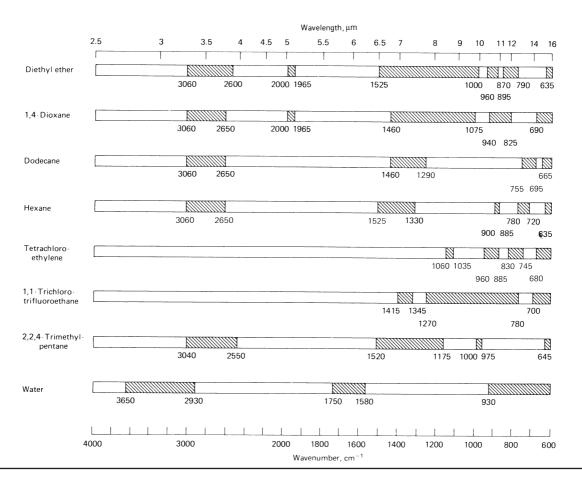
Material	Wavelength range, µm	Wavenumber range, cm ⁻¹	Refractive index at 2 µm
ZnSe, zinc selenide* (vacuum deposited) (Irtran-4)	1–18	10 000–556	2.45
CdTe, cadmium telluride (Irtran-6)	2-28	5 000-360	2.67
Al ₂ O ₃ , sapphire*	0.20-6.5	50 000-1 538	1.76
SiO ₂ , fused quartz	0.16-3.7	62 500-2 700	
Ge, germanium*	0.50-16.7	20 000-600	4.0
Si, silicon*	0.20-6.2	50 000-1 613	3.5
Polyethylene	16–300	625–33	1.54

^{*} Useful for internal reflection work.

TABLE 6.20 Infrared Transmission Characteristics of Selected Solvents







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RAMAN SPECTROSCOPY

Infrared and Raman spectroscopy are related by the fact that both permit the detection of bond vibrations. Like IR spectroscopy, the spectral bands are reported in cm⁻¹. An important difference is that the wavelength and intensity of inelastically scattered light is measured in the Raman spectroscopic method. The "Raman effect" causes the scattered radiation to shift according to the energies of molecular vibrations. Although Raman spectroscopy involves a physical principle different from that in IR spectroscopy, the two techniques are complementary.

Infrared spectroscopy relies on a changing dipole during a bond vibration for absorption of energy to occur. In Raman, it is a change in polarizability in the bond that permits absorption. The simple molecule carbon dioxide, O = C = O, is an instructive example. Both C = O bonds have dipoles but they oppose each other and the net dipole is 0 Debye O(D). The symmetrical stretch in which both O(D) bonds simultaneously extend and contract does not change the dipole but is detectable by Raman because the polarizability of the system alters.

Raman scattering is not a very efficient process and an energy source of considerable power is required. This is typically an argon (Ar) laser. A variety of chemical bonds and systems can be detected by modern Raman spectrometers and typical data are summarized in Tables 6.21–6.30.

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon

Abbreviations Used in the Table

m, moderately strong vw, very weak
m-s, moderate to strong w, weak
m-vs, moderate to very strong w-m, weak to moderately strong
s, strong w-m, weak to moderately strong

vs, very strong w-vs, weak to very strong

Group	Band, cm ⁻¹	Remarks	
	Saturated C—H and C-	-С	
—CH ₃	2969–2967 (s) 2884–2883 (s) ca 1 205 (s) 1150–1135 1060–1056 975–835 (s) 280–220	In aryl compounds In unbranched alkyls In unbranched alkyls Terminal rocking of methyl group CH ₂ —CH ₃ torsion	
—CH ₂ —	2949–2912 (s) 2861–2849 (s) 1473–1443 (m-vs) 1305–1295 (s) 1140–1070 (m) 888–837 (w) 425–150 500–490	Intensity proportional to number of CH ₂ groups Often two bands; see above Substituent on aromatic ring	

 TABLE 6.21
 Raman Frequencies of Single Bonds to Hydrogen and Carbon (continued)

Group	Band, cm ⁻¹	Remarks
	Saturated C—H and C—C	(continued)
—CH(CH ₃) ₂	1350–1330 (m) 835–750 (s)	If attached to C=C bond, 870–800 cm ⁻¹ . If attached to aryl ring, 740 cm ⁻¹
—C(CH ₃) ₃	1265–1240 (m) 1220–1200 (m) 760–685 (vs)	Not seen in <i>tert</i> -butyl bromide Not seen in <i>tert</i> -butyl bromide If attached to C=C or aromatic ring, 760–720 cm ⁻¹
Internal tertiary carbon atom	855–805 (w) 455–410	
Internal quaternary carbon atom	710–680 (vs) 490–470	
Two adjacent tertiary carbon atoms	730–920 770–725	Often a band at 530–524 cm ⁻¹ indicates presence of adjacent tertiary and quaternary carbon atoms.
Dialkyl substitution at α-carbon atom	800–700 (m-s) 680–650 (vs) 605–550	
Cyclopropane	3101–3090 3038–3019 1210–1180 (s)	Shifts to 1 200 cm ⁻¹ for monoalkyl or 1,2-dialkyl substitution and to 1 320 cm ⁻¹ for <i>gem</i> -1,1-dialkyl substitution
Cyclobutane	1 001–960 (vs)	Shifts to 933 cm ⁻¹ for monoalkyl, to 887 cm ⁻¹ for <i>cis</i> -1,3-dialkyl, and to 891 cm ⁻¹ plus 855 cm ⁻¹ (doublet) for <i>trans</i> -1,3-dialkyl subsition
Cyclopentane	900–800 (s)	
Cyclohexane	825–815 (vs) 810–795 (vs)	Boat configuration Chair configuration

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 TABLE 6.21
 Raman Frequencies of Single Bonds to Hydrogen and Carbon (continued)

Group	Band, cm ⁻¹	Remarks
	Saturated C—H and C—C (c	continued)
Cycloheptane	ca 733	
Cyclooctane	ca 703	
CH ₃	1 392–1 377 450–400 (vw) 270–250 (m)	
CH ₃ H C=C CH ₃	1 380–1 379 492–455 (vw) 220–200 (m)	
CH ₃ CH ₃ CH ₃ H	1372–1368 970–952 (m) 592–545 (vw) 420–400 (m) 310–290 (m)	
CH ₃ CH ₃ CH ₃ CH ₃ H	1385–1375 522–488 (w)	
CH ₃ CH ₃ CH ₃ CH ₃	1 392–1 386 690–678 (m-s) 510–485 (m) 424–388 (w)	
>C-C-C€	1 170–1 100 (w-m) 600–580 (m-s)	
>C-C- □ O	1 120–1 090 (m-vs)	Tertiary or quaternary carbon adjacent to carbonyl group lowers the frequency 300 cm ⁻¹
	600–510 (w-m)	
-CH ₂ -CO-	1420–1410 (s)	
—СНО	2850–2810 (m) 2720–2695 (vs)	Often appears as a shoulder

 TABLE 6.21
 Raman Frequencies of Single Bonds to Hydrogen and Carbon (continued)

Group	Band, cm ⁻¹	Remarks
	Unsaturated C—H	
—С≡С—H	3 340–3 270 (w-m)	Alkyl substituents at higher frequencies; unsaturated or aryl substituents at lower frequencies
C=C	3 040–2 995 (m)	
C=C H	3 095–3 050 (m) 2 990–2 983 (s)	Asymmetric $=$ CH ₂ stretch Symmetric $=$ CH ₂ stretch
H R C=C H	1419–1415 (m) 1309–12888 (m)	Plus = CH and = CH stretching bands
H $C=C$ R_1 R_2	1413–1399 (m) 909–885 (m) 711–684 (w)	Plus = CH ₂ stretching bands
R_1 $C=C$ R_2 R_2	1 270–1 251 (m)	Plus = CH stretching band
R_1 $C=C$ H R_2	1314–1290 (m)	Plus = CH stretching band
R_1 $C=C$ R_2 H	1 360–1 322 (w) 830–800 (vw)	Plus = CH stretching band
,	Hydroxy O—H	
Free —OH Intermolecularly bonded Aromatic —OH	3650–3250 (w) 3400–3300 (w) ca 3160 (s)	
—ОН	1 460–1 320 (w) 1 276–1 205 (w-m) 1 260 (w-m)	Common to all OH substituents Primary Secondary

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 TABLE 6.21
 Raman Frequencies of Single Bonds to Hydrogen and Carbon (continued)

Group	Band, cm ⁻¹	Remarks
	Hydroxy O—H (contin	ued)
C—C—OH primary	1 070–1 050 (m-s) 1 030–960 (m-s)	CCO stretching
	480–430 (w-m)	CCO deformation
С—С—ОН		
Secondary	1 135–1 120 (m-s)	
	825–815 (vs)	
	500–490 (w-m)	
Tertiary	1210–1200 (m-s)	
	755–730 (vs)	
	360–350 (w-m)	
—СО—О—Н	1305–1270	CO stretching
	N—H and C—N bor	nds
Amine >N—H		
Associated	3400–3250 (s)	Primary amines show two bands.
Nonbonded	3550–3250 (s)	
Salts	2986–2974	Often obscured by intense CH
		stretching bands
-NH ₂	1650–1590 (w-vs)	Bending
Amides		
Primary	3540–3500 (w)	Both bands lowered ca 150 cm ⁻¹
	3400–3380 (w)	in solid state and H bonding
	1310–1250 (s)	Interaction of NH bending and CN stretching; lowered 50 cm ⁻¹ in nonbonded state
	1 150–1 095 (m)	Rocking of NH ₂
Secondary	3491–3404 (m-s)	Two bands; lowered in frequency
•	` ′	on H bonding and in solid state
	1 190-1 130 (m)	_
	931-865 (m-s)	
	430–395 (w-m)	
	607–555 (m)	O=CN bending
C-N-C	1 070–1 045 (m)	Stretching
		6
≥C-N<		
Primary carbon	1 090–1 060 (m)	CN stretching
Secondary α carbon	1 140–1 035 (m)	Two bands but often obscured. Strong band at 800 cm ⁻¹
Tertiary α carbon	1 240–1 020 (m)	Two bands. Strong band also at 745 cm ⁻¹

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 TABLE 6.22
 Raman Frequencies of Triple Bonds

Abbreviations Used in the Table

m, moderately strong

s-vs, strong to very strong

m, moderately strong s-vs, strong to vs, wery strong vs, very strong

s, strong

Group	Band, cm ⁻¹	Remarks
R—C≡CH	2160-2100 (vs)	Monoalkyl substituted; C≡C
	650–600 (m) 356–335 (s)	C≡CH deformation C≡C—C bending of monoalkyls
$R_1 - C \equiv C - R_2$	2300–2190 (vs)	C≡C stretching of disubstituted alkyls; sometimes two bands
$-C \equiv C - C \equiv C -$	2264–2251 (vs)	
—C≡N	2260–2240 (vs)	Unsaturated nonaryl substituents lower the frequency and enhance the intensity.
	2234–2200 (vs)	Lowered ca 30 cm ⁻¹ with aryl and
	840–800 (s-vs)	conjugated aliphatics CCCN symmetrical stretching
	385–350 (m-s) 200–160 (vs)	Aliphatic nitriles
H—C≡N	2094 (vs)	
Azides —N—N≡N	2 170–2 080 (s) 1 258–1 206 (s)	Asymmetric NNN stretching Symmetric NNN stretching; HN ₃ at 1300 cm ⁻¹
Diazonium salts $R - \stackrel{\scriptscriptstyle{+}}{N} \equiv N$	2300-2240 (s)	
Isonitriles		
$-\overset{\scriptscriptstyle{\dagger}}{\mathrm{N}}\equiv\mathrm{C}^{\scriptscriptstyle{-}}$	2 146–2 134 2 124–2 109	Stretching of aliphatics Stretching of aromatics
Thiocyanates		
—S—C≡N	2260–2240 (vs) 650–600 (s)	Stretching of C≡N Stretching of SC bond

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 TABLE 6.23
 Raman Frequencies of Cumulated Double Bonds

Abbreviations Used in the Table

s, strong vs, very strong vw, very weak w, weak

Group	Band, cm ⁻¹	Remarks	
Allenes			
C=C=C	2000–1960 (s)	Pseudo-asymmetric stretching	
	1080–1060 (vs)	Symmetric stretching	
	356	C=C=C bending	
Carbodiimides (cyanamides)			
-N=C=N-	2 140–2 125 (s)	Asymmetric stretching of aliphatics	
	2150–2100 (vs)	Asymmetric stretching of aromatics; two bands	
	1 460	Symmetrical stretching of aliphatics	
	1150–1140 (vs)	Symmetric stretching of aryls	
Cumulenes (trienes)			
C=C=C=C	2080-2030 (vs)		
	878		
Isocyanates			
-N=C=0	2300-2250 (vw)	Asymmetric stretching	
	1450–1400 (s)	Symmetric stretching	
Isothiocyanates			
-N=C=S	2 2 2 2 0 - 2 1 0 0	Two bands	
	690–650	Alkyl derivatives	
Ketenes			
C=C=0	2060–2040 (vs)	Pseudo-asymmetric stretching	
	1130 (s)	Pseudo-symmetric stretching	
	1374 (s)	Alkyl derivatives	
	1120 (s)	Aryl derivatives	
Sulfinylamines			
R-N=S=0	1306-1214 (w)	Asymmetric stretching	
	1155–989 (s)	Symmetric stretching	

 TABLE 6.24
 Raman Frequencies of Carbonyl Bonds

Abbreviations Used in the Table

m, moderately strong m-s, moderate to strong s, strong s-vs, strong to very strong vs, very strong w, weak

Group	Band, cm ⁻¹	Remarks
Acid anhydrides		
-co-o-co-		
Saturated	1 850–1 780 (m)	
	1771–1770 (m)	
Conjugated, noncyclic	1775	
	1720	
Acid fluorides —CO—F		
Alkyl	1 840–1 835	
Aryl	1812-1800	
Acid chlorides —CO—Cl		
Alkyl	1810–1770 (s)	
Aryl	1774	
•	1731	
Acid bromides —CO—Br		
Alkyl	1812-1788	
Aryl	1775–1754	
Acid iodides —CO—I	1006	
Alkyl	ca 1 806	
Aryl	ca 1752	
Lactones	1850–1730 (s)	
Esters		
Saturated	1741-1725	Alkyl branching on carbon
		adjacent to C=O lowers
		frequency by 5–15 cm ⁻¹ .
Aryl and α , β -unsaturated	1727–1714	
Diesters		
Oxalates	1763–1761	
Phthalates	1738–1728	
C≡C−C0−0−	1716–1708	
Carbamates	1 694–1 688	
Aldehydes	1740–1720 (s-vs)	
Ketones		
Saturated	1725–1700 (vs)	
Aryl	1700-1650 (m)	

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TABLE 6.24 Raman Frequencies of Carbonyl Bonds (continued)

Group	Band, cm ⁻¹	Remarks	
Ketones (continued)			
Alicyclic			
n=4	1782 (m)		
n=5	1744 (m)		
<i>n</i> ≥6	1725–1699 (m)		
Carboxylic acids			
Mono-	1686–1625 (s)	These α -substituents increase the frequency: F, Cl, Br, OH.	
Poly-	1782-1645	Solid state; often two bands	
	1750-1710	In solution; very broad band	
Amino acids	1743–1729		
Carboxylate ions	1690-1550 (w)		
3	1440–1340 (vs)		
Amino acid anion	1743–1729		
	1600-1570 (w)	Often masked by water	
		deformation band near	
		1630 cm ⁻¹	
Amides (see also Table 6.21)			
Primary			
Associated	1686–1576 (m-s)		
	1650–1620 (m)		
Nonbonded	1715–1675 (m)		
	1 620–1 585 (m)		
Secondary	1.600 1.620 ()	D 4 1 (7) 1 (7) 6	
Associated	1680–1630 (w)	Both $cis(Z)$ and $trans(E)$ forms	
	1570–1510 (w)	Trans (E) form	
Nonbonded	1 490–1 440 1 700–1 650	Cis (Z) form	
Nondonaea	1550-1500	Both $cis(Z)$ and $trans(E)$ forms	
Tertiary	1670–1630 (m)	Trans(E) form (no cis band)	
Lactams	1750–1700 (m)		
Lactains	1 /30-1 /00 (III)		

TABLE 6.25 Raman Frequencies of Other Double Bonds

Abbreviations Used in the Table

m, moderately strong m-s, moderate to strong s, strong vs, very strong w, weak

s, strong s-vs, strong to very strong

w-m, weak to moderately strong

Group			Band, cm ⁻¹	Remark	S
			Alkenes >C=C<	<	
>C=C<		1	680–1576 (m-s)	General range	
$ \begin{array}{c c} \hline H & C = C \\ H & H \end{array} $		1	648–1 638 (vs)	C=C stretching	
$ \begin{array}{c c} H & R_1 \\ C = C & R_2 \end{array} $			a 1650 (vs) 70–252 (w)	C=C stretching C=C-C skeletal	deformation
R_1 $C=C$ R_2 R_1 R_2		ca 1660 (vs) 970–952 (w)		C=C stretching Asymmetric CC stretching	
K_1 $C=C$ K_2		1 676–1 665 (s)		C—C stretching	
R_1 $C=C$ R_2 H		1 678–1 664 (vs) 522–488 (w)		C=C stretching C=C-C skeletal	deformation
$ \begin{array}{c c} \hline R_1 \\ \hline R_2 \end{array} $ $ \begin{array}{c c} \hline R_3 \\ \hline H $		1680–1665 (s) 690–678 (m-s) 510–485 (m) 424–388 (w)		C=C stretching Symmetrical CC stretching Skeletal deformation Skeletal deformation	
Haloalkene	X = fluor	ine X = chlorine		X = bromine	X-iodine
		>C=	=C < stretch of halo	oalkanes	
H ₂ C=CHX HXC=CHX	1 654		1603-1601	1596–1593	1 581
$cis(Z)$ $trans(E)$ $H_2C=CX_2$ $X_2C=CHX$	1712 1694 1728 1792		1590–1587 1578–1576 1616–1611 1589–1582	1587–1583 1582–1581 1593 1552	1543 1537
$X_2^{\dagger}C = CX_2$	1872		1577–1571	1 547	1465 (solid)

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TABLE 6.25 Raman Frequencies of Other Double Bonds (*continued*)

Group	Band, cm ⁻¹	Remarks
	>C—N—bonds	
Aldimines (azomethines) H $C=N-R_2$	1673–1639	Dialkyl substituents at higher frequency; diaryl substituents at lower end of range
R_1	1405–1400 (s)	at lower ond of range
Aldoximines and Ketoximes >C—N—OH	1680–1617 (vs) 1335–1330 (w)	
Azines >C=N-N=C<	1 625–1 608 (s)	
Hydrazones $ \begin{array}{ccc} H & H \\ C = N - N \\ R_1 & R_2 \end{array} $	1660–1610 (s-vs)	
Imido ethers O C=NH	1658-1648	NH stretching at 3360–3327 cm ⁻¹
Semicarbazones and thiosemicarbazones H C=N-N NH ₂ C O (or S)	1665–1642 (vs) 1620–1610 (vs)	Aliphatic. Thiosemicarbazones fall in lower end of range. Aromatic derivatives
	Azo compounds —N=	-N—
	1580-1570 (vs) 1442-1380 (vs) 1060-1030 (vs)	Nonconjugated Conjugated to aromatic ring CN stretching in aryl compounds
	Nitro compounds N=	=0
Alkyl nitrites	1660–1620 (s)	N=O stretching
Alkyl nitrates	1635–1622 (w-m) 1285–1260 (vs) 610–562 (m)	Asymmetric NO ₂ stretching Symmetric NO ₂ stretching NO ₂ deformation

TABLE 6.25 Raman Frequencies of Other Double Bonds (*continued*)

Group	Band, cm ⁻¹	Remarks	
	Nitro compounds N=O (a	continued)	
Nitroalkanes			
Primary	1 560–1 548 (m-s)		
. ,	1395–1370 (s)	Sensitive to substituents attached to CNO ₂ group	
	915–898 (m-s)	10 01 02 group	
	894–873 (m-s)		
	618–609 (w)		
	640–615 (w)	Shoulder	
	494–472 (w-m)	Broad; useful to distinguish from secondary nitroalkanes	
Secondary	1553–1547 (m)	,	
•	1375–1360 (s)		
	908-868 (m)		
	863–847 (s)		
	625–613 (m)		
	560–516 (s)	Sharp band	
Tertiary	1 543–1 533 (m)		
	1 355–1 345 (s)		
Nitrogen oxides			
$\geqslant \dot{N} \rightarrow \bar{O}$	1612–1602 (s)		
211 70	1 252 (m)		
	1 049–1 017 (s)		
	835 (s)		
	541 (w)		
	469 (w)		

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 TABLE 6.26
 Raman Frequencies of Aromatic Compounds

Abbreviations Used in the Table

m, moderately strong m-s, moderate to strong

m-vs, moderate to strong

s, strong

s-vs, strong to very strong

var, of variable strength

vs, very strong w, weak

w-m, weak to moderately strong

Group	Band, cm ⁻¹	Remarks
	Common features	
Aromatic compounds	3 070–3 020 (s) 1 630–1 570 (m-s)	CH stretching C—C stretching
	Substitution patterns of the ber	nzene ring
Monosubstituted	1 180–1 170 (w-m) 1 035–1 015 (s) 1 010–990 (vs) 630–605 (w)	Characteristic feature; found also with 1,3- and 1,3,5-substitutions
1,2-Disubstituted	1 230–1 215 (m) 1 060–1 020 (s) 740–715 (m)	Characteristic feature Lowered 60 cm ⁻¹ for halogen substituents
1,3-Disubstituted	1010–990 (vs) 750–640 (s)	Characteristic feature
1,4-Disubstituted	1 230–1 200 (s-vs) 1 180–1 150 (m) 830–750 (vs) 650–630 (m-w)	Lower frequency with Cl substituents
Isolated hydrogen	1 379 (s-vs) 1 290–1 200 (s) 745–670 (m-vs) 580–480 (s)	Characteristic feature
1,2,3-Trisubstituted	1100–1050 (m) 670–500 (vs) 490–430 (w)	The lighter the mass of the substituent, the higher the frequency
1,2,4-Trisubstituted	750–650 (vs) 580–540 (var) 500–450 (var)	Lighter mass at higher frequencies

TABLE 6.26 Raman Frequencies of Aromatic Compounds (*continued*)

Group	Band, cm ⁻¹	Remarks		
Subst	itution patterns of the benzene	ring (continued)		
1,3,5-Trisubstituted	1010–990 (vs)			
Completely substituted	1 296 (s) 550 (vs) 450 (m) 361 (m)			
	Other aromatic compou	inds		
Naphthalenes	1390-1370 1026-1012 767-762 535-512 519-512	Ring breathing α or β substituents β substituents α substituents β substituents β substituents		
Disubstituted naphthalenes	hthalenes 773–737 (s) 726–705 (s) 690–634 (s) 608 575–569 544–537 1,2-; 1,3-; 2,3-; 2,6 1,3-; 1,4-(two bands) 1,2-; 1,4-(two bands) 1,2-; 1,4-(two bands) 1,3- 1,2-; 1,3-; 1,6- 1,2-; 1,7-; 1,8-			
Anthracenes	1415–1385	Ring breathing		

TABLE 6.27 Raman Frequencies of Sulfur Compounds

Abbreviations Used in the Table

Abbierunions	Osea in the Tubic
m, moderately strong	s-vs, strong to very st

trong m-s, moderate to strong vs, very strong w-m, weak to moderately strong s, strong

Group	Band, cm ⁻¹	Remarks
—S—H	2590–2560 (s)	SH stretching for both aliphatic and aromatic
>C=S	1 065–1 050 (m) 735–690 (vs)	Solid state
>S=0 In (RO ₂) ₂ SO In (R ₂ N) ₂ SO	1 209–1 198 1 108	One or two bands

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TABLE 6.27 Raman Frequencies of Sulfur Compounds (continued)

Group	Band, cm ⁻¹	Remarks
> S =O (continued) In R ₂ SO SOF ₂ SOCl ₂ SOBr ₂	1 070–1 010 (w-m) 1 308 1 233 1 121	Broad
—SO ₂ —	1 330–1 260 (m-s) 1 155–1 110 (s) 610–540 (m) 512–485 (m)	Asymmetric SO ₂ stretching Symmetric SO ₂ stretching Scissoring mode of aryls Scissoring mode of alkyls
	ca 1322 (m) 1163–1138 (s) 524–510 (s)	Asymmetric SO ₂ stretching Symmetric SO ₂ stretching Scissoring mode
	1 363–1 338 (w-m) 1 192–1 165 (vs) 589–517 (w-m)	SO ₂ stretching. Aryl substituents occur at higher range. Scissoring (two bands). Aryl substituents occur at higher range of frequencies.
SO ₂ _S_	1 334–1 305 (m-s) 1 128–1 126 (s) 559–553 (m-s)	
X—SO ₂ —X	1412–1361 (w-m) (F) (CI) 1263–1168 (s) (F) (CI) 596–531 (s)	
	1388–1372 (s) 1196–1188 (vs)	
-0-C-S-	670–620 (vs) 480–450 (vs)	C=S stretching CS stretching
≥C—SH	920 (m) 850–820 (m)	C—SH deformation of aryls
≥C-S-	752 (vs), 731 (vs) 742–722 (m-s) 698 (w), 678 (s) 693–639 (s) 651–610 (s-vs) 589–585 (vs)	With vinyl group attached With CH ₃ attached With allyl group attached Ethyl or longer alkyl chain Isopropyl group attached tert-Butyl group attached

TABLE 6.27 Raman Frequencies of Sulfur Compounds (*continued*)

Group	Band, cm ⁻¹	Remarks
\ge C—S—(continued)		
$(CH_2)_n$ S		
n=2	1112	
n = 4	688	
n = 5	659	
\geqslant C $-(S-S)_n$ $-C \leqslant$	715–620 (vs)	Two bands; CS stretching
	525–510 (vs)	Two bands; SS stretching
Didi-n-alkyl disulfides	576 (s)	CS stretching
Di-tert-butyl disulfide	543 (m)	SS stretching
Trisulfides	510–480 (s)	SS stretching

TABLE 6.28 Raman Frequencies of Ethers

Abbreviations Used in the Table

m, moderately strong s, strong

var, of variable strength vs, very strong

Group	Band, cm ⁻¹	Remarks
⇒C−0−C€ Aliphatic	1 200–1 070 (m)	Asymmetrical COC stretching. Symmetrical substitution gives
	930–830 (s) 800–700 (s)	higher frequencies Symmetrical COC stretching Branching at α carbon gives higher frequencies.
Aromatic	550–400 1310–1210 (m) 1050–1010 (m)	ingitet requesions.
≥C-0-C-0-C€	1 145–1 129 (m) 900–800 (vs) 537–370 (s) 396–295	
>C C<	1 280–1 240 (s)	Ring breathing
-0-0-	800–770 (var)	
(CH2)n O	1040–1010 (s) 920–900 (s) 820–800 (s)	

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 TABLE 6.29
 Raman Frequencies of Halogen Compounds

Abbreviations Used in the Table

m-s, moderate to strong s, strong

var, of variable strength vs, very strong

Group	Band, cm ⁻¹	Remarks		
С—F	1400–870	Correlations of limited applicability because of vibrational coupling with stretching		
C—Cl Primary Secondary Tertiary	350–290 (s) 660–650 (vs) 760–605 (s) 620–540 (var)	CCCl bending; general May be one to four bands May be one to three bands		
=C-Cl	844–564 438–396 381–170			
=CCl ₂	601–441 300–235			
C—Br	690–490 (s)	Often several bands; primary at higher range of frequencies. Tertiary has very strong band at ca 520cm ⁻¹ .		
	305–258 (m-s)			
=C-Br	745–565 356–318 240–115			
=CBr ₂	467–265 185–145			
C—I	663–595 309 154–85			
=C—I	ca 180	Solid state		
=CI ₂	ca 265 ca 105	Solid state Solid state		

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TABLE 6.30 Raman Frequencies of Miscellaneous Compounds

Abbreviations Used in the Table

m, moderately strong s, strong

vs, very strong vvs, very very strong

		<u> </u>
Group	Band, cm ⁻¹	Remarks
C—As	570–550 (vs)	CAs stretching
	240–220 (vs)	CAsC deformation
C—Pb	480–420 (s)	CPb stretching
С—Нд	570–510 (vvs)	CHg stretching
C—Si	1300–1200 (s)	CSi stretching
C—Sn	600–450 (s)	CSn stretching
Р—Н	2350-2240 (m)	PH stretching
	Heterocyclic ring	s
Trimethylene oxide	1029	
Trimethylene imine	1026	
Tetrahydrofuran	914	
Pyrrolidine	899	
1,3-Dioxolane	939	
1,4-Dioxane	834	
Piperidine	815	
Tetrahydropyran	818	
Morpholine	832	
Piperazine	836	
Furan	1515-1460	2-Substituted
	1140	
Pyrazole	1040–990	
Pyrrole	1420–1360 (vs)	
·	1144	
Thiophene	1410(s)	
•	1365 (s)	
	1085 (vs)	
	1035 (s)	
	832 (vs)	
	610 (s)	
Pyridine	1030 (vs)	
-	990 (vs)	

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Nuclear Magnetic Resonance (NMR) Spectroscopy is by far the most widely used analytical technique in the modern organic chemistry lab. Numerous monographs have been written on this subject. It would be impossible to cover all of the significant points here. The reader who is interested in knowing what the proton (¹H) or carbon (¹³C) spectrum of a particular compound is directed to the Aldrich Library of NMR Spectra or the Sadtler Library.

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A number of resources are also available online. These include software for the prediction and analysis of spectral data and databases. Resources include:

Proton NMR basics:

http://jchemed.chem.wisc.edu/JCESoft/Programs/PNMRB/

NMR database:

www.acornnmr.com/database.htm

NMR prediction:

www.acdlabs.com/products/spec lab/predict nmr/

NMR library:

www.acdlabs.com/products/spec_lab/exp_spectra/spec_libraries/aldrich.html

NMR Periodic Table for half-integer quadrupole spins:

www.pascal-man.com/periodic-table/periodictable.html

Nuclear Magnetic Resonance

Table 6.31 presents the nuclear properties of the elements. Hydrogen (¹H) is an almost ideal nucleus for NMR spectroscopy. First, its natural abundance is high so most of the nuclei present in the sample will be detected in the NMR experiment. Second, its sensitivity is high meaning that its signal is readily detected. The nuclei that have been most generally used in organic chemistry are ¹H and ¹³C although the natural abundance of the latter is low. Advances in instruments have made the acquisition of ¹³C-NMR spectra routine. Several other nuclei have high natural abundance and occur frequently in organic compounds. These include ⁷Li, ¹¹B, ¹⁴N, ¹⁹F, ²³Na, and ³⁵Cl, which are shown in bold type in Table 6.31. Modern NMR spectrometers permit the acquisition of NMR spectra from many nuclei depending on the probe. The most favorable nuclei are those that have spin 1/2, high natural abundance, high sensitivity, and no quadrupole moment. Of course, the importance of the problem under study will ultimately dictate whether the investigator will invest the time and effort to obtain the spectrum when the experiment is difficult.

Table 6.31 Nuclear properties of the elements

In the following table the magnetic moment μ is in multiples of the nuclear magneton $\mu_N(eh/4\pi Mc)$ with diamagnetic correction, the spin I is in multiples of $h/2\pi$, and the electric quadrupole moment Q is in multiples of 10^{-28} square meters. Nuclei with spin $\frac{1}{2}$ have no quadrupole moment. The sign of μ and Q is uncertain for those nuclides for which no sign is given. Sensitivity is for equal number of nuclei at constant field. NMR frequency at any magnetic field is the entry for column 5 multiplied by the value of the magnetic field in kilogauss. For example, in a magnetic field of 14.0924 kG, protons (1 H) will precess at a frequency of 4.25760×14.0924 kG = 60.000 MHz. In a magnetic field of 23.4924 kG, protons will precess at 4.25760×23.4924 kG = 100.00 MHz.

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 TABLE 6.31
 Nuclear Properties of the Elements

Nuclide	Natural abundance,	Spin I	Sensitivity at constant field relative to ¹ H	NMR frequency for a 1000 G field, MHz	Magnetic moment μ/μ_N , J·T ⁻¹	Electric quadrupole moment <i>Q</i> , 10^{-28} m ²
¹n		-1/2	0.322	2.91670	-1.91312	_
1H	99.985	1/2	1.000	4.257 60	+2.79278	_
² H	0.015	1	0.00964	0.653 57	+0.85742	+0.0028
³ H		1/2	1.21	4.54131	+2.9789	_
³ He	0.00013	-1/2	0.443	3.24338	-2.1276	_
⁶ Li	7.42	1	0.00851	0.62655	+0.82203	-0.0008
⁷ Li	92.58	3/2	0.294	1.65465	+3.25636	-0.04
9Be	100	-3/2	0.0139	0.59827	-1.17745	0.05
$^{10}{ m B}$	19.7	3	0.0199	0.4574	+1.8006	+0.111
11 B	80.3	3/2	0.165	1.36595	+2.6885	+0.041
¹³ C	1.108	1/2	0.0159	1.07054	+0.7024	_
^{14}N	99.635	1	0.00101	0.3076	+0.40375	+0.01
^{15}N	0.365	-1/2	0.00104	0.4315	-0.2831	_
¹⁷ O	0.037	-5/2	0.0291	0.57739	-1.8937	-0.004
19 F	100	1/2	0.834	4.00543	+2.6288	_
²¹ Ne	0.257	-3/2	0.0272	0.33611	-0.66176	+0.09
²² Na	_	3	0.0181	0.4434	1.746	_
²³ Na	100	3/2	100	1.12621	+2.21740	+0.10
²⁴ Na	_	4	0.00115	0.322	1.690	_
^{25}Mg	10.11	-5/2	0.0268	0.2606	-0.8554	+0.22
²⁷ Al	100	5/2	0.207	1.10940	+3.6413	+0.15
²⁹ Si	4.71	-1/2	0.0785	0.8458	-0.55526	_
31 P	100	1/2	0.0664	1.7238	+1.1317	_
33 S	0.76	3/2	0.00226	0.3266	+0.6435	-0.055
³⁵ S	_	3/2	0.00850	0.508	_	+0.038
35Cl	75.53	3/2	0.00471	0.4171	+0.82181	-0.080
³⁶ Cl	_	2	0.0121	0.4893	+1.2853	-0.10
³⁷ Cl	24.47	3/2	0.00272	0.3472	+0.68407	-0.0062
³⁹ K	93.22	3/2	0.000508	0.19864	+0.39143	+0.049
⁴⁰ K	0.0118	4	0.00521	0.2470	-1.2981	-0.061
⁴¹ K	6.77	3/2	0.0000839	0.10903	+0.2149	+0.060
⁴³ Ca	0.145	7/2	0.0639	0.28654	-1.3172	
⁴⁵ Sc ⁴⁷ Ti	100	7/2	0.301	1.03434	+4.7559	-0.22
'' 11 ⁴⁹ Ti	7.32	-5/2	0.00210	0.23997	-0.78846	+0.29
50V	5.46 0.25	-7/2 6	0.00376	0.24004	-1.10414	+0.24
51 V	99.75	7/2	0.0553 0.383	0.4243	+3.3470 +5.1485	0.06 -0.05
⁵³ Cr	99.75	3/2	0.383	1.11922 0.24063	+3.1483 -0.4735	-0.03 +0.03
55Mn	100	5/2	0.178	1.05542	+3.449	+0.03
⁵⁷ Fe	2.17	1/2	0.0000333	0.138	+0.09042	+0.4 —
⁵⁹ Co	100	7/2	0.281	1.0072	+4.616	+0.38
⁶¹ Ni	1.25	3/2	0.00350	0.38048	-0.7498	+0.36
⁶³ Cu	69.1	3/2	0.00330	1.1285	+2.2228	-0.211
⁶⁵ Cu	30.9	3/2	0.0938	1.2090	+2.3812	-0.195
⁶⁷ Zn						
						+0.19
⁶⁷ Zn ⁶⁹ Ga	4.11 60.2	5/2 3/2	0.00286 0.0693	0.2663 1.02188	+0.87524 +2.0145	+0.16

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TABLE 6.31 Nuclear Properties of the Elements 9 (continued)

Nuclide	Natural abundance,	Spin I	Sensitivity at constant field relative to ¹ H	NMR frequency for a 1000 G field, MHz	Magnetic moment μ/μ_N , J·T ⁻¹	Electric quadrupole moment <i>Q</i> , 10^{-28} m ²
⁷¹ Ga	39.8	3/2	0.142	1.29840	+2.5597	+0.12
⁷⁵ As	100	3/2	0.0251	0.7292	+1.439	+0.29
⁷⁷ Se	7.58	1/2	0.00697	0.8118	+0.534	_
⁷⁹ Br	50.52	3/2	0.0786	1.0669	+2.1055	+0.37
81 Br	49.48	3/2	0.0984	1.1498	+2.2696	+0.31
87Rb	27.85	3/2	0.177	1.2923	+2.7500	+0.13
⁹³ Nb	100	9/2	0.482	1.04048	+6.167	-0.22
^{113}In	4.23	-1/2	0.345	0.9312	-0.6225	_
¹¹⁹ Sn	8.58	-1/2	0.0518	1.5868	-1.0461	_
¹²¹ Sb	57.25	5/2	0.160	1.0192	+3.3592	-0.28
¹²³ Sb	42.75	7/2	0.0457	0.5519	+2.5466	-0.36
¹²⁵ Te	6.99	-1/2	0.0316	1.3453	-0.8872	_
^{127}I	100	5/2	0.0935	0.8517	+2.8091	-0.79
¹²⁹ Xe	26.44	-1/2	0.0212	1.17779	-0.7768	_
¹⁹⁵ Pt	33.8	1/2	0.00994	0.91523	+0.6022	_
¹⁹⁹ Hg	16.84	1/2	0.00572	0.7612	+0.50415	_
²⁰³ Tl	29.50	1/2	0.187	2.4332	+1.6115	_
207Pb	21.7	1/2	0.00913	0.8898	10.5783	_

Chemical Shifts

In essence, the chemical shift of a nucleus such as proton (1H) is its resonance frequency. It is usually expressed in parts per million (ppm) relative to a standard. The most common standard is tetramethylsilane [(CH₃)₄Si, TMS] which defines 0 on the delta (δ) scale and 10 on the older, less used τ scale. A small amount of TMS is typically added to the NMR solution to be examined. The presence of an internal standard minimizes experimental variations. This is particularly important because the chemical shift is typically a change of only a few hertz per megahertz, hence the part per million (ppm) scale. The separation of peaks will be greater in hertz at higher field but spectra obtained at different field strengths are comparable on the ppm scale. Common reference standards are listed in Table 6.32.

 TABLE 6.32
 Proton Chemical Shifts of Reference Compounds Relative to Tetramethylsilane

Compound	Chemical shift δ , ppm*	Solvent(s)
Tetramethylsilane, (CH ₃) ₄ Si	0.0	CDCl ₃ , CCl ₄
3-(Trimethylsilyl)-1-propanesulfonic acid, sodium salt (DSS), (CH ₃) ₃ SiCH ₂ CH ₂ COONa	0.0	D_2O
Sodium acetate	1.90	D_2O
1,2-Dibromoethane	3.63	CDCl ₃

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TABLE 6.32 Proton Chemical Shifts of Reference Compounds Relative to Tetramethylsilane (continued)

Compound	Chemical shift δ , ppm*	Solvent(s)
1,1,2,2-Tetrachloroethane, Cl ₂ HCCHCl ₂	5.95	CDCl ₃ , CCl ₄
1,4-Benzoquinone	6.78	CDCl ₃ , CCl ₄
1,4-Dichlorobenzene	7.23	CCl ₄
Chloroform, CHCl ₃	7.27	CDCl ₃ , CCl ₄
Benzene	7.37	CDCl ₃ , CCl ₄
1,3,5-Trinitrobenzene	9.21	DMSO- d_6 †
		CDCl ₃

^{*}Shift relative to TMS, first entry in table; † Dimethylsulfoxide-d₆

A typical solution prepared for NMR analysis rarely contains more than a few percent of solute. Thus, protons on the solvent could significantly distort the spectrum. When ¹H-NMR are desired, solvents having no protons (CS₂ or CCl₄) or deuterated solvents are used. Table 6.33 gives the common NMR solvents used. Although modern manufacturing methods typically produce NMR solvents having high isotopic purity, incomplete deuteration of a protonic solvent will result in a residual signal.

TABLE 6,33 Common NMR Solvents

Solvent	Detail	Group*	δ (ppm)
Acetic acid- d_4	D ₃ C—COOD	CD₂H	2.05
		OH	11.5†
Acetone- d_6	CD ₃ COCD ₃	CD_2H	2.057
Acetonitrile- d_3	$CD_3C \equiv N$	CD_2H	1.95
Benzene-d ₆	C_6D_6	С—Н	6.78
$tert$ -Butanol- d_1	(CH ₃) ₃ COD	CD_2H	1.28
Chloroform- d_1	Cl ₃ CD	Cl ₃ CH	7.25
Cyclohexane-d ₁₂	C_6D_{12}	CHD	1.40
Deuterium oxide	D_2O	HOD	4.7†
Dimethylformamide- d_7	$(CD_3)_2N$ — CD = O	CD_2H	2.75; 2.95
		-CH=O	8.05
Dimethylsulfoxide-d ₆	CD_3SOCD_3	CD_2H	2.51
$(DMSO-d_6)$	0.		
	D_2C CD_2 D_2C CD_2	Absorbed H ₂ O	3.3†
$1,4$ -Dioxane- d_8	$D_2C_CCD_2$	Methylene	3.55
Hexamethylphosphoramide- d_{18} , HMPA- d_{18} , HMPT- d_{18}	$(D_3C)_2N - P - N(CD_3)_2$ $N(CD_3)_2$	Methyl	2.60
Methanol- d_{Λ}	CD ₃ OD	CD ₂ H	3.35
141Ct11a11O1-u ₄	CD ₃ OD	OH	4.8†

^{*}Impurity peak resulting from incomplete deuteration or exchange.

[†]These values may vary greatly depending on the solute and its concentration.

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TABLE 6.33 Common NMR Solvents (*continued*)

Solvent	Detail	Group*	$\delta(ppm)$
Dichloromethane- d_2 Pyridine- d_5	Cl ₂ CD ₂ D(4)	Cl ₂ CDH C-2—H	5.35 8.5
	$\bigcup_{D} \bigvee_{N} \bigcup_{D(2)}^{D(3)}$	C-3—H C-4—H	7.0 7.35
Tetrahydrofuran-d ₆	$D_2C - CD_2$ $D_2C - CD_2$	CD-2—H CD-3—H	3.58 1.73
Toluene- d_8	$\begin{array}{c} D \\ D \\ \end{array}$	$\mathrm{CD_2H}$ Ring CD	2.3 7.1
Trifluoroacetic acid- d_1	F ₃ C—COOD	Hydroxyl	11.3†

^{*}Impurity peak resulting from incomplete deuteration or exchange. †These values may vary greatly depending on the solute and its concentration.

TABLE 6.34 Proton Chemical Shifts

Values are given on the δ scale; $\tau = 10.00 - \delta$.

Abbreviations Used in the Table
R, alkyl group
Ar, aryl group

Substituent group	Methyl protons	Methylene protons	Methine proton
HC—C—CH ₂	0.95	1.20	1.55
HC—C—NR ₂	1.05	1.45	1.70
HC-C-C=C	1.00	1.35	1.70
HC-C-C=O	1.05	1.55	1.95
HC—C—NRAr	1.10	1.50	1.80
HC-C-H(C=O)R	1.10	1.50	1.90
$HC-C-(C=O)NR_2$	1.10	1.50	1.80
HC-C-(C=O)Ar	1.15	1.55	1.90
HC-C-(C=O)OR	1.15	1.70	1.90
HC—C—Ar	1.15	1.55	1.80
НС—С—ОН	1.20	1.50	1.75
HC-C-OR	1.20	1.50	1.75
$HC-C-C\equiv CR$	1.20	1.50	1.80
$HC-C-C\equiv N$	1.25	1.65	2.00
HC-C-SR	1.25	1.60	1.90
HC—C—OAr	1.30	1.55	2.00
HC-C-O(C=O)R	1.30	1.60	1.80
HC—C—SH	1.30	1.60	1.65
HC-C-(S=O)R			
and $HC - C - SO_2R$	1.35	1.70	
$HC-C-NR_3^+$	1.40	1.75	2.05

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TABLE 6.34 Proton Chemical Shifts (*continued*)

Substituent group	Methyl protons	Methylene protons	Methine proton
HC-C-O-N=0	1.40		
$HC-C-O(C=O)CF_3$	1.40	1.65	
HC-C-Cl	1.55	1.80	1.95
HC—C—F	1.55	1.85	2.15
HC-C-NO ₂	1.60	2.05	2.50
HC-C-O(C=O)Ar	1.65	1.75	1.85
HC—C—I	1.75	1.80	2.10
HC—C—Br	1.80	1.85	1.90
HC—CH ₂	0.90	1.30	1.50
HC-C=C	1.60	2.05	
HC—C≡C	1.70	2.20	2.80
HC-(C=O)OR	2.00	2.25	2.50
$HC-(C=O)NR_2$	2.00	2.25	2.40
HC—SR	2.05	2.55	3.00
HC-O-O	2.10	2.30	2.55
HC-(C=O)R	2.10	2.35	2.65
HC—C≡N	2.15	2.45	2.90
HC—I	2.15	3.15	4.25
НС—СНО	2.20	2.40	
HC—Ar	2.25	2.45	2.85
HC—NR ₂	2.25	2.40	2.80
HC—SSR	2.35	2.70	
HC—(C=O)Ar	2.40	2.70	3.40
HC—SAr	2.40		
HC—NRAr	2.60	3.10	3.60
HC — SO_2R and HC — $(SO)R$	2.60	3.05	
HC—Br	2.70	3.40	4.10
HC—NR ₃ ⁺	2.95	3.10	3.60
HC-NH(C=O)R	2.95	3.35	3.85
HC—SO ₃ R	2.95		2.02
HC—Cl	3.05	3.45	4.05
HC—OH and HC—OR	3.20	3.40	3.60
HC—PAr ₃	3.20	3.40	2.00
HC—NH ₂	3.50	3.75	4.05
HC-O(C=O)R	3.65	4.10	4.95
HC—OAr	3.80	4.00	4.60
HC—O(C=O)Ar	3.80	4.20	5.05
HC—O(C=O)CF	3.95	4.30	
HC—F	4.25	4.50	4.80
HC—NO ₂	4.30	4.35	4.60
Cyclopropane		0.20	0.40
Cyclobutane		2.45	0.10
Cyclopentane		1.65	
Cyclohexane		1.50	1.80
Cycloheptane		1.25	1.00
Cycloneptane		1.43	

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 TABLE 6.34
 Proton Chemical Shifts (continued)

Substituent group	Proton shift	Substituent group	Proton shift
НС≡СН	2.35	HO-C=0	10–12
HC≡CAr	2.90	HO—SO ₂	11-12
$HC \equiv C - C = C$	2.75	HO—Ar	4.5-6.5
HAr	7.20	HO—R	0.5-4.5
HCO—O	8.1	HS—Ar	2.8-3.6
HCO-R	9.4–10.0	HS—R	1–2
HCO—Ar	9.7–10.5	HN—Ar	3–6
HO-N=C (oxime)	9–12	HN—R	0.5–5

Saturated heterocyclic ring systems

TABLE 6.34 Proton Chemical Shifts (*continued*)

Substituent group	Methyl protons	Methylene protons	Methine proton
	Unsatu	rated cyclic systems	
6.3 7.4	7.5 N 8.5	7.4 7.6 8.0 N 8.8	7.8
6.1 N H	7.6 N 9.2	7.6 7.5 7.9 9.1 8.5 N	8.3 7.9
S 7.2	7.1 N 9.2	7.8 O 7.0 O	8.1 N ⁺ O ⁻
8.0 N 7.4 S	N N 8.5	7.9 0 0 0	\$\begin{align*} \begin{align*} \begi
7.2 7.2 HN N	NH	6.3 6.5 7.3 N	4.5

TABLE 6.35 Estimation of Chemical Shift for Protons of —CH₂— and >CH— Groups

 $\delta_{\text{CH}_2} = 0.23 + C_1 + C_2$ $\delta_{\text{CH}} = 0.23 + C_1 + C_2 + C_3$

X*	С	X*	C	X*	C
$\begin{array}{c} -\text{CH}_3 \\ -\text{CF}_3 \\ > \text{C} - \text{C} < \\ -\text{C} \equiv \text{C} - \text{R} \\ -\text{COOR} \\ -\text{NR}_2 \\ -\text{CONR}_2 \end{array}$	0.5 1.1 1.3 1.4 1.5 1.6	—SR —C≡C—Ar —CN —CO—R —I —Ph —Br	1.6 1.7 1.7 1.7 1.8 1.8 2.3	-OR -Cl -OH -N=C=S -OCOR -OPh	2.4 2.5 2.6 2.9 3.1 3.2

^{*}R, alkyl group; Ar, aryl group; Ph, phenyl group.

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TABLE 6.36 Estimation of Chemical Shift of Proton Attached to a Double Bond

Positive Z values indicate a downfield shift, and an arrow indicates the point of attachment of the substituent group to the double bond.

$$\delta_{C=C} = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$$

$$R_{cis} \qquad H$$

$$C=C$$

$$R_{none} \qquad T_{none}$$

R	Z_{gem} , ppm	Z_{cis} , ppm	Z_{trans} , ppm
\rightarrow H	0	0	0
→alkyl	0.45	-0.22	-0.28
→alkyl—ring (5- or 6-member)	0.69	-0.25	-0.28
\rightarrow CH ₂ O—	0.64	-0.01	-0.02
\rightarrow CH ₂ S $-$	0.71	-0.13	-0.22
\rightarrow CH ₂ X (X: F, Cl, Br)	0.70	0.11	-0.04
\rightarrow CH ₂ N $<$	0.58	-0.10	-0.08
C=C (isolated)	1.00	-0.09	-0.23
C = C (conjugated)	1.24	0.02	-0.05
→C≡N	0.27	0.75	0.55
\rightarrow C \equiv C $-$	0.47	0.38	0.12
C=O (isolated)	1.10	1.12	0.87
C=O (conjugated)	1.06	0.91	0.74
→COOH (isolated)	0.97	1.41	0.71
→COOH (conjugated)	0.80	0.98	0.32
→COOR (isolated)	0.80	1.18	0.55
→COOR (conjugated)	0.78	1.01	0.46
$ \begin{array}{c} H \\ \rightarrow C = O \end{array} $	1.02	0.95	1.17
→C=0	1.37	0.98	0.46
Cl	1.11	1.46	1.01
→OR (R: aliphatic)	1.22	-1.07	-1.21
→OR (R: conjugated)	1.21	-0.60	-1.00
→OCOR	2.11	-0.35	-0.64
$\rightarrow CH_2 - \stackrel{ }{C} = 0; \rightarrow CH_2 - C \equiv N$	0.69	-0.08	-0.06
→CH ₂ —aromatic ring	1.05	-0.29	-0.32
→F	1.54	-0.40	-1.02
→Cl	1.08	0.18	0.13
→Br	1.07	0.45	0.55
\rightarrow I	1.14	0.81	0.88
→N—R (R: aliphatic)	0.80	-1.26	-1.21
→N —K (K: aliphatic)	0.80	-1.26	-1.21

TABLE 6.36 Estimation of Chemical Shift of Proton Attached to a Double Bond (*continued*)

R	Z_{gem} , ppm	Z_{cis} , ppm	Z_{trans} , ppm
$ \xrightarrow{\mid} N - R (R: conjugated) $	1.17	-0.53	-0.99
$\rightarrow N-C=O$	2.08	-0.57	-0.72
→aromatic	1.38	0.36	-0.07
$\rightarrow CF_3$	0.66	0.61	0.32
\rightarrow aromatic (o-substituted)	1.65	0.19	0.09
→SR	1.11	-0.29	-0.13
\rightarrow SO ₂	1.55	1.16	0.93

TABLE 6.37 Chemical Shifts in Monosubstituted Benzene

 $\delta = 7.27 + \Delta_i$

Substituent	Δ_{ortho}	$\Delta_{\it meta}$	$\Delta_{\it para}$
NO_2	0.94	0.18	0.39
CHO	0.58	0.20	0.26
COOH	0.80	0.16	0.25
COOCH ₃	0.71	0.08	0.20
COCI	0.82	0.21	0.35
CCl ₃	0.8	0.2	0.2
COCH ₃	0.62	0.10	0.25
CN	0.26	0.18	0.30
CONH ₂	0.65	0.20	0.22
NH ₃	0.4	0.2	0.2
CH ₂ X*	0.0-0.1	0.0-0.1	0.0-0.1
CH ₃	-0.16	-0.09	-0.17
CH ₂ CH ₃	-0.15	-0.06	-0.18
CH(CH ₃) ₂	-0.14	-0.09	-0.18
$C(CH_3)_2$	-0.09	0.05	-0.23
F	-0.30	-0.02	-0.23
Cl	0.01	-0.06	-0.08
Br	0.19	-0.12	-0.05
I	0.39	-0.25	-0.02
NH_2	-0.76	-0.25	-0.63
OCH ₃	-0.46	-0.10	-0.41
OH	-0.49	-0.13	-0.2
OCOR	-0.2	0.1	-0.2
NHCH ₃	-0.8	-0.3	-0.6
$N(CH_3)_2$	-0.60	-0.10	-0.62
	1	1	

^{*}X = Cl, alkyl, OH, or NH₂.

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TABLE 6.38 Proton Spin Coupling Constants

Structure	J, Hz	Structure		J, Hz
Н		н	cis (Z)	2
·c′		H N	trans (E)	6
/ \ _H	12–15		gem	4
			2-3	1.8
CH-CH (free rotation)	6–8	4 3	3-4	3.5
		5 1 2	2-4	0-1
>CH-OH (no exchange)	5	0	2-5	1–2
>CH-NH	4–8		2-3	5–6
CH—SH	6–8	4 7 3	3-4	3.5-5.0
/ ,,		5 2	2-4	1.5
H \		3	2-5	3.4
CH-C=0	1–3		0	6–12
/		$\langle \bigcirc \rangle$ F	m	4–8
H		H	p	1.5-2.5
-N=C	8–16		_	2.5
ЪН	0–3	$\langle \bigcirc \rangle$ -CH ₃	o m	1.5
H _t H _g gem		F	p	0
C=C $cis(Z)$	6–14		Ρ	
H_c H $trans(E)$	11–18	H		8–10
H_c H $trans(E)$		/~~/_H	a-a a-e	2–3
H_c CH $cis(Z)$	0.5-3	Н	e-e	2–3
C = C trans (E)	0.5–3		C C	2 3
	4–10	Cyclopentane	e cis (7)	4–6
H' _t `H _g gem	4-10		rans (E)	4–6
	10–13	Cyclobutane		8
>C=CH-CH=C<	10-13			8
=CH-C=O	6		rans (E)	9–11
H	0	Cyclopropan	rans (E)	9–11 6–8
			gem	4–6
-CH ₂ -C≡C-CH	0-3	(6–10
>CH-C≡CH `	0–3	√ √н	o m	1–3
H H 3-member	0–2		p	0–1
C-C 4-member	2–4	` `н	Ρ	
5-member	5–7			
(ring) 6-member	6–9	2	1-2	8–9
7-member	10–13	3	2-3	6
oin (7)	4–5			5–6
cis(Z)	3	4	2-3	3–6 7–9
trans (E) gem	5 5–6	'()	3-4	1–2
cis (Z)		6 2	2-4	1-2
S cis (Z) / trans (E)	0	19	3-5	
gem	7 6		2-5 2-6	0–1 0–1
	Ü		2-0	0-1

TABLE 6.38 Proton Spin Coupling Constants (continued)

Structure	J, Hz	Structure	J, Hz
3 1-2 1-3 2-3 3-4	2–3 2–3 2–3 3–4	$\begin{array}{c c} H_t & gem \\ C = C & cis(Z) \\ H_c & F & trans(E) \end{array}$	72–90 -3 to 20 12–40
2-4 2-5	1–2 1–3	C=C CH ₃	2–4
C F	45–52	C=C H HC≡CF	0–6 21
CH-CF gauche trans (Z)	0–12 10–45	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	34 12 <5-8

TABLE 6.39 Carbon-13 Chemical Shifts

Values given in ppm on the δ scale, relative to tetramethylsilane

Substituent group	Primary carbon	Secondary carbon	Tertiary carbon	Quaternary carbon
Alkanes				
C-C	5-30	25-45	23–58	28-50
C—O	45-60	42–71	62–78	73–86
C—N	13-45	44–58	50-70	60–75
C—S	10-30	22–42	55–67	53-62
C—halide (I to Cl)	3–25	3–40	34–58	35–75
Substituent group	δ, ppm	Substituent	t group	δ, ppm
Cyclopropane	-5-5	Alcohols R	Alcohols R—OH	
Cycloalkane C ₄ –C ₁₀	5–25	Ethers R—	Ethers R—O—R	
Mercaptanes	5–70	Nitro R—1	Nitro R—NO ₂	
Amines		Alkynes	Alkynes	
R_2N-C	20–70	HC≡C	HC≡CR	
Aryl—N	128-138	RC≡C!	RC≡CR	
Sulfoxides, sulfones	35–55	Acetals, ke	Acetals, ketals	
Thiocyanates R—SCN	96–118	Esters	Esters	
Alkenes		Saturate	Saturated	
$H_2C =$	100-122	α,β-Uns	α,β -Unsaturated	
R ₂ C=	110-150	Isocyanide	Isocyanides R—NC	

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TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Substituent group	δ, ppm	Substituent group	δ, ppm
Heteroaromatics		Carboxylic acids	
C=N	100-152	Nonconjugated	162-165
C_{α}	142-160	Conjugated	165-184
Cyanates R—OCN	105-120	Salts (anion)	175–195
Isocyanates R—NCO	115-135	Ketones	
Isothiocyanates R—NCS	115-142	α-Halo	160-200
Nitriles, cyanides	117-124	Nonconjugated	192-202
Aromatics		α,β -Unsaturated	202-220
Aryl-C	125-145	Imides	165-180
Aryl-P	119-128	Acyl chlorides R—CO—Cl	165-183
Aryl-N	128-138	Thioureas	165-185
Aryl-O	133–152	Aldehydes	
Azomethines	145-162	α-Halo	170-190
Carbonates	159-162	Nonconjugated	182-192
Ureas	150-170	Conjugated	192-208
Anhydrides	150-175	Thioketones R—CS—R	190-202
Amides	154–178	Carbonyl M(CO),	190-218
Oximes	155–165	Allenes = C=	197–205

Saturated heterocyclic ring systems

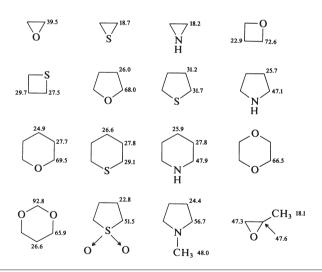


TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Unsaturated cyclic systems

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TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Saturated alicyclic ring systems

TABLE 6.40 Estimation of Chemical Shifts of Alkane Carbons

Relative to tetramethylsilane

Positive terms indicate a downfield shift.

$$\delta_C = -2.6 + 9.1 n_\alpha + 9.4 n_\beta - 2.5 n_\gamma + 0.3 n_\delta + 0.1 n_\epsilon$$
 (plus any correction factors)

where n_{α} is the number of carbons bonded directly to the *i*th carbon atom and n_{β} , n_{γ} , n_{δ} , and $n_{\& epsilon}$; are the number of carbon atoms two, three, four, and five bonds removed. The constant is the chemical shift for methane

Chain branching*	Correction factor	Chain branching*	Correction factor
1°(3°)	-1.1	4°(1°)	-1.5
1°(4°)	-3.4	2°(4°)	-7.2
2°(3°)	-2.5	3°(3°)	-9.5
3°(2°)	-3.7	4°(2°)	-8.4

^{*1°} signifies a CH₃— group; 2°, a —CH₂— group; 3°, a \Rightarrow CH— group; and 4°, a \Rightarrow C \leqslant group. 1°(3°) signifies a methyl group bound to a \Rightarrow CH— group, and so on.

$$\begin{split} \textit{Examples} : \text{For 3-methyl pentane, CH}_3 &- \text{CH}_2 - \text{CH(CH}_3) - \text{CH}_2 - \text{CH}_3, \\ \delta_{C=2} &= -2.6 + 9.1(2) + 9.4(2) - 2.5 - 1(1)[2^\circ(3^\circ)] = 29.4 \\ \delta_{C=3} &= -2.6 + 9.1(3) + 9.4(2) + (2)[3^\circ(2^\circ)] = 36.2 \end{split}$$

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 TABLE 6.41
 Effect of Substituent Groups on Alkyl Chemical Shifts

These increments are added to the shift value of the appropriate carbon atom as calculated from Table 6.40.

	α carbon		eta carbon		
Substituent group Y*	Straight	Branched	Straight	Branched	γ carbon
—со—он	20.9	16	2.5	2	-2.2
—COO ⁻ (anion)	24.4	20	4.1	3	-1.6
—CO—OR	20.5	17	2.5	2	-2
-co-cl	33	28		2	
-CO-NH ₂	22	2.5			-0.5
—СНО	31		0		-2
-co-R	30	24	1	1	-2
—OH	48.3	40.8	10.2	7.7	-5.8
—OR	58	51	8	5	-4
-O-CO-NH ₂	51		8		
-O-CO-R	51	45	6	5	-3
-C-CO-Ar	53				
—F	68	63	9	6	-4
—Cl	31.2	32	10.5	10	-4.6
—Br	20.0	25	10.6	10	-3.1
—I	-8	4	11.3	12	-1.0
$-NH_2$	29.3	24	11.3	10	-4.6
NH ₃ +	26	24	8	6	-5
—NHR	36.9	31	8.3	6	-3.5
$-NR_2$	42		6		-3
$-NR_3^+$	31		5		-7
$-NO_2$	63	57	4	4	
—CN	4	1	3	3	-3
—SH	11	11	12	11	-6
—SR	20		7		-3
$-CH=CH_2$	20		6		-0.5
$-C_6H_5$	23	17	9	7	-2
—С≡СН	4.5		5.5		-3.5

^{*}R, alkyl group; Ar, aryl group.

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TABLE 6.42 Estimation of Chemical Shift of Carbon Attached to a Double Bond

The olefinic carbon chemical shift is calculated from the equation

$$\delta_C = 123.3 + 10.6n_\alpha + 7.2n_\beta - 7.9n_{\alpha'} - 1.8n_{\beta'}$$
 (plus any steric correction terms)

where n is the number of carbon atoms at the particular position, namely,

$$\beta \quad \alpha \quad \alpha' \quad \beta'$$
 $C-C=C-C$

Substituents on both sides of the double bond are considered separately. Additional vinyl carbons are treated as if they were alkyl carbons. The method is applicable to alicyclic alkenes; in small rings carbons are counted twice, that is, from both sides of the double bond where applicable. The constant in the equation is the chemical shift for ethylene. The effect of other substituent groups is tabulated below.

Substituent group	β	α	α'	β΄
—OR	2	29	-39	-1
—ОН	6			-1
$-O-CO-CH_3$	-3	18	-27	4
—CO—CH ₃		15	6	
—СНО		13.6	13.2	
—СО—ОН		5.2	9.1	
—CO—OR		6	7	
—CN		-15.4	14.3	
—F		24.9	-34.3	
—Cl	-1	3.3	-5.4	2
—Br	0	-7.2	-0.7	2
—I		-37.4	7.7	
$-C_6H_5$		12	-11	
			Steric correct	ion
Substituent pair			term	
α, α'	trans (E)		0	
α,α'	cis(Z)		-1.1	
α,α	gem		-4.8	
α',α'			+2.5	
β , β			+2.3	
- · -	1	1	. 2.0	

SPECTROSCOPY 6.89

TABLE 6.43 Carbon-13 Chemical Shifts in Substituted Benzenes

 $\delta_{\rm C} = 128.5 + \Delta$

Substituent group	Δ_{C-1}	Δ_{ortho}	Δ_{meta}	Δ_{para}
—CH ₃	9.3	0.8	-0.1	-2.9
-CH ₂ CH ₃	15.6	-0.4	0	-2.6
—CH(CH ₃) ₂	20.2	-2.5	0.1	-2.4
$-C(CH_3)_3$	22.4	-3.1	-0.1	-2.9
$-CH_2O-CO-CH_3$	7.7	0	0	0
$-C_6H_5$	13.1	-1.1	0.4	-1.2
-CH=CH	9.5	-2.0	0.2	-0.5
—C≡CH	-6.1	3.8	0.4	-0.2
—CH₂OH	12.3	-1.4	-1.4	-1.4
—со—он	2.1	1.5	0	5.1
—COO ⁻ (anion)	8	1	0	3
—CO—OCH ₃	2.1	1.1	0.1	4.5
—CO—CH ₃	9.1	0.1	0	4.2
—СНО	8.6	1.3	0.6	5.5
—CO—Cl	4.6	2.4	1	6.2
—CO—CF ₃	-5.6	1.8	0.7	6.7
$-CO-C_6H_5$	9.4	1.7	-0.2	3.6
—CN	-15.4	3.6	0.6	3.9
—ОН	26.9	-12.7	1.4	-7.3
—OCH ₃	31.4	-14.0	1.0	-7.7
$-OC_6H_5$	29.2	-9.4	1.6	-5.1
$-O-CO-CH_3$	23.0	-6.4	1.3	-2.3
-NH ₂	18.0	-13.3	0.9	-9.8
$-N(CH_3)_2$	22.4	-15.7	0.8	-11.5
$-N(C_6H_5)_2$	19	-4	1	-6
−NHC ₆ H ₅	14.6	-10.7	0.7	-7.7
$-NH-CO-CH_3$	11.1	-9.9	0.2	-5.6
$-NO_2$	20.0	-4.8	0.9	5.8
—F	34.8	-12.9	1.4	-4.5
—Cl	6.2	0.4	1.3	-1.9
—Br	-5.5	3.4	1.7	-1.6
—I	-32.2	9.9	2.6	-1.4
—CF ₃	-9.0	-2.2	0.3	3.2
-NCO	5.7	-3.6	1.2	-2.8
—SH	2.3	1.1	1.1	-3.1
−SCH ₃	10.2	-1.8	0.4	-3.6
$-SO_2-NH_2$	15.3	-2.9	0.4	3.3
—Si(CH ₃) ₃	13.4	4.4	-1.1	-1.1

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TABLE 6.44 Carbon-13 Chemical Shifts in Substituted Pyridines* $\delta_c(k) = C_k + \Delta_i$

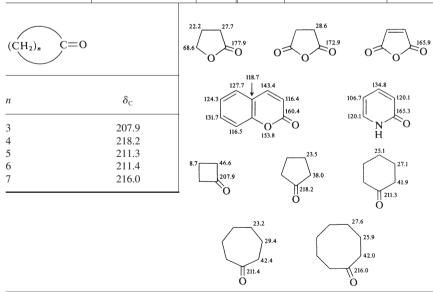
Substituent group	$C_2 = C_6 = 14$ $\Delta_{C-2} \text{ or } \Delta_C$		Δ_{23}	Δ_{24}		Δ_{25}		Δ_{26}
	9.1 14.0 4.3 3.5 14.9 15.3 11.3 8.0 -15.8 14.4 2.3 -6.7		-1.0 -2.1 -2.8 -2.6 -17.2 -13.1 -14.7 -5.1 5.0 -14.7 0.7 4.8	-0.1 0.7 1.3 0.4 2.1 2.3 5.5 -1.7 5.1 3.3 3.3	- - -	-3.4 -3.1 3.0 4.1 -7.5 10.6 6.6 3.6 -2.7 -1.2 -0.5		-0.1 0.2 -0.2 0.7 -6.8 -2.2 -0.9 0.4 1.9 -1.7 0.6 1.4
Substituent group	Δ_{32}		$= C_5 = 124$ $= C_5 = 124$ $= 3$ or Δ_{C-1}	Δ_{34}		Δ_{35}		
	1.3 0.3 0.5 2.4 -10.7 -11.9 3.6 -0.3 2.1 7.1		9.0 15.0 -0.3 7.9 31.4 21.5 -13.7 8.2 -2.6 -28.4	0.2 -1.5 -3.7 0 -12.2 -14.2 4.4 -0.2 2.9 9.1	-	-0.8 -0.3 -2.7 0.6 1.3 0.9 0.6 0.7 1.2 2.4		-2.3 -1.8 4.2 5.4 -8.6 -10.8 4.2 -1.4 -0.9
Substituent group	$\Delta_{42} = \Delta_{46}$			$\Delta_{43} = \Delta_{45}$		C		136.2
-CH ₃ -CH ₂ CH ₃ -CH=CH ₂ -CO-CH ₃ -CHO -NH ₂ -CN -Br	0.5 0 0.3 1.6 1.7 0.9 2.1 3.0		0.8 -0.3 -2.9 -2.6 -0.6 -13.8 2.2 3.4			1 -1	0.8 5.9 8.6 6.8 5.5 9.6 5.7 3.0	

^{*}May be used for disubstituted, polyheterocyclic, and polynuclear systems if deviations due to steric and mesomeric effects are allowed for.

TABLE 6.45 Carbon-13 Chemical Shifts of Carbonyl Group

$$\overset{O}{\overset{\parallel}{X-C-Y}}$$

X	Y	$\delta_{ m C}$	X	Y	$\delta_{\scriptscriptstyle m C}$
н—	—CH ₃	199.7	CH ₃ —	-CH=CH ₂	196.9
Н—	—CCl ₃	175.3		—C ₆ H ₅	197.6
Н—	-NH ₂	165.5	CH ₃ —	$-CH_2-CO-CH_3$	201.9
Н—	—N(CH ₃) ₂	162.4			(keto) 191.4 (enol)
н—	2-Furyl	153.3	CH ₃ —	—СН,СНО	167.7
Н—	2-Pyrrolyl	134.0	CH ₃ —	$-C_6H_5$ -CH ₃	196 (m, p)
H—	2-Thienyl	143.3			199 (o)
(CH ₃) ₂ CH—	—OH	184.8	CH ₃ —	$-2,6-(CH_3)_2C_6H_5$	206
C ₆ H ₅ —	—ОН	172.6	CH ₃ —	—ОН	178
CF ₃ —	—ОН	163.0	CH ₃ —	—O ⁻ (anion)	181.5
CCl ₃ —	—ОН	168.0	CH ₃ —	—OCH ₃	170.7
CH ₃ CH(NH ₂)—	—ОН	176.5	CH ₃ —	$-O-CH=CH_2$	167.7
CF ₃ —	−OCH ₂ CH ₃	158.1	CH ₃ —	—O—CH(CH ₃) ₂	170.3
H_2N —	−OCH ₂ CH ₃	157.8	CH ₃ —	-O-CO-CH ₃	167.3
2-Furyl	−OCH ₃	159.1	CH ₃ —	-NH ₂	172.7
(CH ₃) ₂ N—	$-C_6H_5$	170.8	CH ₃ —	−NHCH ₃	172
CH ₂ =CHCH ₂ O-			CH ₃ —	$-N(CH_3)_2$	169.5
CO—	-OCH ₂ CH=CH ₂	157.6	CH ₃ —	—Cl	169.6
CH ₃ CH ₂ —	−CH ₂ CH ₃	211.4	CH ₃ —	—Br	165.6
CH ₃ —CH ₂ —	-O-CO-CH ₂ CH ₃	170.3	CH ₃ —	—I	158.9
CH ₃ —	—СH ₃	205.8			
CH ₃ —	-CH ₂ CH ₃	207			



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TABLE 6.46 One-Bond Carbon–Hydrogen Spin Coupling Constants

Structure	J_{CH} , Hz	Structure	J_{CH} , Hz
H—CH ₃	125.0	H _t H _g gem	177
H—CH ₂ CH ₃	124.9	C=C $cis(Z)$	163
CH_3 — CH_2 — CH_3	119.2		
H — $C(CH_3)_2$	114.2	H_c CN trans (E)	165
H—CH ₂ CH ₂ OH	126.9		162
$H-CH_2CH=CH_2$	122.4	H OH cis (Z)	163
H — $CH_2C_6H_5$	129.4	C=N trans (E)	177
$H-CH_2C\equiv CH$	132.0	CII	
H—CH ₂ CN	136.1	CH ₃	
H — $CH(CN)_2$	145.2		
H—CH ₂ —halogen	149–152	$H-CH=O; CH_3-\underline{CH}=O$	172
H — CHF_2	184.5	H_2N — CH = O	188.3
H—CHCl ₂	178.0	$(CH_3)_2N-\underline{CH}=O$	191
H — CH_2NH_2	133.0	Н—СООН	222
H — $CH_2NH_3^+$	145.0	H—COO ⁻ (anion)	195
H — CH_2OH (or H — CH_2OR)	140–141	H—CO—OCH ₃	226
H — $CH(OR)_2$	161–162	H—CO—F	267
H — $C(OR)_3$	186	CH ₃ CH ₂ —O— <u>CH</u> O	225.6
H — $C(OH)R_2$	143	Cl ₃ —CHO	207
H — CH_2NO_2	146.0	H—C≡CH	249
H — $CH(NO_2)_2$	169.4	H—C≡CCH ₃	248
H—CH ₂ COOH	130.0	$H-C \equiv CC_6H_5$	251
H—CH(COOH) ₂	132.0	H—C≡CCH ₂ OH	241
$H-CH=CH_2$	156.2	H—CN	269
$H-C(CH_3)=C(CH_3)_2$	148.4	Cyclopropane	161
H — CH = $C(tert$ - $C_4H_9)_2$	152	Cyclobutane	136
H — $C(tert$ - $C_4H_9)$ =		Cyclopentane	131
$C(tert-C_4H_9)_2$	143	Cyclohexane	123
Methylenecycloalkane	150 155	Tetrahydrofuran 2,5	149
C_4 – C_7	153–155	3,4	133
$H-CH=C=CH_2$	168	1,4-Dioxane	145
$H-C(C_6H_5)=CH(C_6H_5)$	1.55	Benzene	159
cis(Z)	155	Fluorobenzene 2,6	155
trans(E)	151	3,5	163
Cyclopropene	220	4	161
	200	Bromobenzene 2,6	171
H_t H_g gem	200	3,5	164
C=C $cis(Z)$	159	4	161
H_c F trans (E)	162	Benzonitrile 2,6	173
		3,6	166
H_t H_g gem	195	4	163
C=C cis (Z)	163	Nitrobenzene 2,6	171
H _c C1 trans (E)	161	3,5	167
H_t , H_g gem		4	163
	162	Mesitylene	154
C=C $cis(Z)$	157	2,6	170
H_c CHO trans (E)	162	3,5	163
	102	N 4	152
		·	

TABLE 6.46 One-Bond Carbon–Hydrogen Spin Coupling Constants (*continued*)

Structure		$J_{ m CH},{ m Hz}$	Structure	J_{CH} , Hz
2,4,6-Trimethylp	yridine	158	N.	
$\left\langle \begin{array}{c} N\\ N\\ H \end{array} \right\rangle$	2,5 3,4	183 170	N 2 4 H	208 199
	2,5 3,4	201 175	N N H	205
S	2,5 3,4	185 167	N-N N	216
N H	3,5 4	190 178	H	

 TABLE 6.47
 Two-Bond Carbon–Hydrogen Spin Coupling Constants

Structure	$^2J_{\mathrm{CH}}$, Hz	Structure	² <i>J</i> _{CH} , Hz
$\begin{array}{c} \underline{CH_3-CH_2-H} \\ \underline{CCI_3-CH_2-H} \\ \underline{CCI_3-CH_2-H} \\ \underline{CICH_2-CH_2CI} \\ \underline{CI_2CH-CHCI_2} \\ \underline{CH_3-CHO} \\ \underline{CH_3-CHO} \\ \underline{CH_3-CHO} \\ \underline{CCH_3)_2\underline{C}=O} \\ \underline{CH_2-CH_2-CHO} \\ \underline{CC_2-CH-CHO} \\ \underline{CC_2-CH-CHO} \\ \underline{H_2NCH-CHO} \\ \underline{CHO} \\$	-4.5 5.9 -3.4 1.2 26.7 -2.4 5.5 26.9 26.9 6.0 20.0 1.0	$(CH_2)_n C = CH_2 n = 4$ $n = 5$ $H $	4.2 5.2 5.5 16.0 0.8 49.3 61.0 33.2 32.5 35.3 46.3
C_6H_6	1.0	$C_{6}H_{5}-C\equiv\underline{C}\equiv C\underline{H}_{3}$	10.8

 TABLE 6.48
 Carbon–Carbon Spin Coupling Constants

Structure*	$J_{\rm CC}$, Hz	Structure*	$J_{\rm CC},{ m Hz}$
H ₃ C—CH ₃ H ₃ C—CHR ₂	35 37	H ₃ C—CH ₂ NH ₂ C—C=O	37 38–40
H ₃ C—CH ₂ Ar	34	$\underline{\mathbf{C}} - \underline{\mathbf{C}} - \mathbf{C} = 0$	36
H ₃ C—CH ₂ CN H ₃ C—CH ₂ —CH ₂ OH	33	$C-CO-Ar$ $C-CO-O^-$ (anion)	43 52
C-1, C-2 C-2, C-3	38 34	C—CO—N C—CO—OH	52 57

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TABLE 6.48 Carbon–Carbon Spin Coupling Constants (*continued*)

Structure*	$J_{\rm CC}$, Hz	Structure*	$J_{\rm CC}$, Hz
C—CO—OR	59	C ₆ H ₅ NH ₂	
C—CN	52-57	1–2	61
$C - C = C^2 J_{CC} = 11.8$	67	2–3	58
$H_2C = CH_2$	68	3–4	57
$\geq \underline{\mathbf{C}} = \underline{\mathbf{C}} - \mathbf{CO} - \mathbf{OH}$	70–71	$^{3}J_{2-5}$	7.9
$\geq \underline{\mathbf{C}} = \underline{\mathbf{C}} - \mathbf{C}\mathbf{N}$	71	C ₆ H ₅ CH ₃	44
$\geq \underline{\mathbf{C}} = \underline{\mathbf{C}} - \mathbf{Ar}$	67–70	Pyridine	
C_6H_6	57	2–3	54
$C_6H_5NO_2$		3–4	56
1–2	55	$^{3}J_{2-5}$	14
2-3, 3-4	56	Furan	69
$^{3}J_{2-5}$	7.6	Pyrrole	69
C_6H_5I		Thiophene	64
1–2	60	$H_2\underline{C} = \underline{C} = C(CH_3)_2$	100
2–3	53	_C≡C—	170–176
3–4	58		
$^{3}J_{2-5}$	8.6	Structure	$^{2}J_{\mathrm{CC}},\mathrm{Hz}$
C ₆ H ₅ —OCH ₃			
2–3	58	CH ₃ —CO—CH ₃	16
3–4	56	$CH_3-CO-\underline{C}H_3$ $CH_3-C\equiv CH$	11.8
		$CH_3-C=CH$ CH_3CH_2-CN	33
		$\underline{\underline{c}}_{13}\underline{c}_{12}\underline{-\underline{c}}_{1N}$	33

^{*} R, alkyl group; Ar, aryl group.

 TABLE 6.49
 Carbon–Fluorine Spin Coupling Constants

Structure*	J_{CF} , Hz	Structure*	J_{CF} , Hz
F H C H	-158	F F CH ₃	-271
F H		F H	-165
FH	-235	H Ar F-CH ₂ CH ₂ - or F-CR ₃	-167
F F	-274	$p ext{-}F ext{-}C_6H_4 ext{-}OR$ $p ext{-}F ext{-}C_6H_4 ext{-}R$ $p ext{-}F ext{-}C_6H_4 ext{-}CF_3$ $p ext{-}F ext{-}C_6H_4 ext{-}CO ext{-}CH_3$	-237 -241 -252 -253
F F	-259	$p\text{-F}\text{C}_6\text{H}_4\text{NO}_2$ $F\text{C}_6\text{H}_5$ $^2J_{\text{CF}}=21.0$ $^3J_{\text{CF}}=7.7$	-257 -244
F		$^4J_{\rm CF} = 3.4$	

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TABLE 6.49 Carbon–Fluorine Spin Coupling Constants (*continued*)

Structure*	$J_{\scriptscriptstyle{\mathrm{CF}}}$, Hz	Structure*	$J_{\rm\scriptscriptstyle CF}$, Hz
F C=CH ₂	-287	F H C CH ₂ OH	-241
F C=O	-308	F F CH ₂ OH	-278
F C=O	-353	F F C OCF ₃	-265
F C=O	-369	F F CO-CH ₃	-289

^{*} Ar, aryl group; R, alkyl group.

TABLE 6.50 Carbon-13 Chemical Shifts of Deuterated Solvents *Relative to tetramethylsilane*

Solvent	Group	δ, ppm
Acetic- d_3 acid- d_1	Methyl	20.0
	Carbonyl	205.8
Acetone- d_6	Methyl	28.1
-	Carbonyl	178.4
Acetonitrile-d ₃	Methyl	1.3
	Carbonyl	117.7
Benzene- d_6		128.5
Carbon disulfide		193
Carbon tetrachloride		97
Chloroform- d_1		77
Cyclohexane-d ₁₂		25.2
Dimethyl sulfoxide- d_6		39.5
1,4-Dioxane- d_6		67
Formic acid- d_1	Carbonyl	165.5
Methanol- d_4		47–49
Methylene chloride- d_2		53.8
Nitromethane- d_3		57.3
Pyridine-d ₅	C_3, C_5	123.5
-	C_4	135.5
	$C_3, C_5 \\ C_4 \\ C_2, C_6$	149.9

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 TABLE 6.51
 Carbon-13 Spin Coupling Constants with Various Nuclei

Nuclei	Structure	¹ <i>J</i> , Hz	²J, Hz	³J, Hz	⁴J, Hz
² H	CDCl ₃	32			
	CD ₃ —CO—CD ₃	20			
	$(CD_3)_2SO$	22			
	C_6D_6	26			
⁷ Li	CH ₃ Li	15			
11 B	$(C_6H_5)_4B^-$	49		3	
^{14}N	$(CH_3)_4N^+$	10			
	CH ₃ NC	8			
²⁹ Si	(CH ₃) ₄ Si	52			
31 P	$(CH_3)_3P$	14			
	$(C_4H_9)_3P$	11	12	5	
	$(C_6H_5)_3P$	12	20	7	0
	$(CH_3)_4P^+$	56			
	$(C_4H_9)_4P^+$	48	4	15	
	$(C_6H_5)_4P^+$	88	11	13	3
	$R(RO)_2P = O$	142	5–7		
	$(C_4H_9O)_3P = O$		6	7	
⁷⁷ Se	$(CH_3)_2Se$	62			
	$(CH_3)_3Se^+$	50			
¹¹³ Cd	(CH ₃) ₂ Cd	513, 537			
¹¹⁹ Sn	(CH ₃) ₄ Sn	340			
	$(CH_3)_3SnC_6H_5$	474	37	47	11
¹²⁵ Te	$(CH_3)_2$ Te	162			
¹⁹⁹ Hg	$(CH_3)_2Hg$	687			
	$(C_6H_5)_2Hg$	1186	88	102	18
²⁰⁷ Pb	$(CH_3)_2Pb$	250			
	$(C_6H_5)_4Pb$	481	68	81	20

TABLE 6.52 Boron-11 Chemical Shifts

Values given in ppm on the δ scale, relative to $B(OCH_3)_3$

Structure	δ , ppm	Structure	δ, ppm
R ₃ B	−67 to −68	C ₆ H ₅ BCl ₂	-36
Ar ₃ B	-43	$C_6H_5B(OH)_2$	-14
BF ₃	24	$C_6H_5B(OR)_2$	-10
BCl ₃	-12	M(BH ₄)	55-61
BBr ₃	-6	$B(BF_4)$	19–20
BI_3	41		
B(OH) ₃	36	NH—BH	
$B(OR)_3$	0–1	HB NH	-12
$B(NR_2)_3$	-13	NH—BH	

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TABLE 6.52 Boron-11 Chemical Shifts (*continued*)

Structure	δ, ppm	Structure	δ, ppm
H, H, H		R ₂ O(or ROH) · BCl ₃	−7 to −8
B	37	$R_2O(or\ ROH) \cdot BBr_3$	23–24
H N H R_2		$R_2O(or ROH) \cdot BI_3$	74–82
H NR ₂ H	15	N·BBr,	24
R B B			
H NR ₂ ' H		Boranes	
$(CH_3)_2N$ — $B(CH_3)_2$	62	B_2H_6	1
Addition complexes		B_4H_{10}	
$R_2O \cdot BH_3$	18-19	(BH ₂)	25
$R_3N \cdot BH_3$	25	(BH)	60
$R_2NH \cdot BH_3$	33		Base Apex
$N \cdot BH_3$	31	B₅H ₉	31 70
$R_2O(\text{or ROH}) \cdot BF_3$	17–19	$\begin{array}{c c} B_5H_{11} \\ B_{10}H_{14} \end{array}$	$ \begin{array}{c cc} -16 & 50 \\ 7 & 54 \end{array} $

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts *Values given in ppm on the* δ *scale, relative to NH*₃*liquid*

Substituent group	δ, ppm	Substituent group	δ, ppm
Aliphatic amines		Ureas	
Primary	1-59	Aliphatic	63-84
Secondary	7–81	Aryl	105-108
Tertiary	14-44	Sulfonamides	79-164
Cyclo, primary	29–44	Amides	
Aryl amines	40–100	HCO—NHR	
Aryl hydrazines	40–100	R = primary	100-115
Piperidines,		R = secondary	104-148
decahydroquinolines	30–82	R = tertiary	96-133
Amine cations		HCO—NH—Aryl	138-141
Primary	19–59	RCO—NHR or	103-130
Secondary	40–74	RCO—NR ₂	
Tertiary	30–67	RCO—NH—Aryl	131-136
Quaternary	43–70	Aryl—CO—H—Aryl	ca 126
Enamines, tertiary type		Guanidines	
Alkyl	29–82	Amino	30-60
Cycloalkyl	55-104	Imino	166-207
Aminophosphines	59-100	Thioureas	85-111
Amine N-oxides	95–122	Thioamides	135–154

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TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*continued*)

Substituent group	δ, ppm	Substituent group	δ , ppm
Cyanamides		Diazo	
R ₂ N—	-12 to -38	Internal	226-303
—CN	175-200	Terminal	315-440
Carbodiimides	95-120	Nitrilium ions	123-150
Isocyanates		Azinium ions	185-220
Alkyl, primary	14-32	Azine N-oxides	230-300
Alkyl, secondary and tertiary	54-57	Nitrones	270-285
Aryl	ca 46	Imides	170-178
Isothiocyanates	90-107	Imimes	310-359
Azides	52-80	Oximes	340-380
	108-122	Nitramines	
	240-260	Amine	252-280
Lactams	113-122	-NO ₂	328-355
Hydrazones		Nitrates	310-353
Amino	141-167	gem-Polynitroalkanes	310-353
Imino	319-327	Nitro	
Cyanates	155-182	Aryl	350-382
Nitrile N-oxides, fulminates	195-225	Alkyl	372-410
Isonitriles		Hetero, unsaturated	354-367
Alkyl, primary	162-178	Azoxy	330-356
Alkyl, secondary	191-199	Azo	504-570
Aryl	ca 180	Nitrosamines	222-250
Nitriles			525-550
Alkyl	235-241	Nitrites	555-582
Aryl	258-268	Thionitrites	720-790
Thiocyanates	265-280	Nitroso	
Diazonium		Aliphatic amines, NO	535-560
Internal	222-230	Aryl	804-913
Terminal	315-322	-	

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (continued

Substituent group	δ, ppm	Substituent group	δ, ppm
	Saturated c	yclic systems	
$(CH_2)_n$ N—H $n=2$	-8.5	H	35.5
n = 3 n = 4 n = 5 O	25.3 36.7 37.7 32.1	N H N H	$7.5 \\ (\text{in C}_6\text{H}_6) \\ 18.0 \\ (\text{in H}_2\text{O})$
		cis (Z) trans (E)	42.4 52.9
	Unsaturated	cyclic systems	

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TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*continued*)

Unsaturated cyclic systems (continued) X δ ,ppm O 517 S 331 Se 373 N 293 N' 281 316 361 330 412 N H 114 283 308 N 280 351 261

 TABLE 6.54
 Nitrogen-15 Chemical Shifts in Monosubstituted Pyridine

 $\delta = 317.3 + \Delta_i$

Substituent	$\Delta_{ ext{C-}2}$	$\Delta_{ ext{C-3}}$	$\Delta_{C\text{-}4}$
—СН3	-0.4	0.3	-8.0
-CH ₂ CH ₃	-1.8		-6.6
-CH(CH ₃) ₂	-5.1		-5.9
—C(CH ₃) ₃	-2.5		-5.8
—CN	-0.9	-0.8	10.6
—СНО	10	11	29
−CO−CH ₃	-9	15	11
—CO—OCH ₂ CH ₃	11.8		-5
−OCH ₃	-49	0	-23
—ОН	-126	-2	-118
$-NO_2$	-23	1	22
$-NH_2$	-45	10	-46
—F	-42	-18	
—Cl	-4	4	-6
—Br	2	8	7

TABLE 6.55 Nitrogen-15 Chemical Shifts for Standards

Values given in ppm, relative to NH3 liquid at 23 °C

Substance	δ, ppm	Conditions
Nitromethane (neat)	380.2	For organic solvents and acidic aqueous solutions
Potassium (or sodium) nitrate (saturated aqueous solution)	376.5	For neutral and basic aqueous solutions
$C(NO_2)_4$	331	For nitro compounds
(CH ₃) ₂ —CHO (neat)	103.8	For organic solvents and aqueous solutions
$(C_2H_5)_4N^+Cl^-$	64.4	Saturated aqueous solution
(CH ₃) ₄ N ⁺ Cl ⁻	43.5	Saturated aqueous solution
NH ₄ Cl	27.3	Saturated aqueous solution
NH ₄ NO ₃	20.7	Saturated aqueous solution
NH ₃	0.0	Liquid, 25°C
	-15.9	Vapor, 5 atm

TABLE 6.56 Nitrogen-15 to Hydrogen-1 Spin Coupling Constants

Structure	J, Hz	Structure	J, Hz
R—NH ₂ and R ₂ NH Aryl—NH ₂ p-CH ₃ O—aryl—NH ₂ p-O ₂ N—aryl—NH ₂ Amine salts (alkyl and aryl) Aryl—NHOH Aryl—NHCH ₃ Aryl—NHCH ₂ F Aryl—NHNH ₂ p-O ₂ N—aryl—NHNH ₂ Aryl—SO ₂ —NH ₂ Aryl—SO ₂ —NHR O H 3yn (to -CO-) C-N H H anti	61–67 78 79 90–93 73–76 79 87 90 90 99 81 86 88	O H C-N R R Pyrrole $HC \equiv NH^+$ $> P-NH_2$ $(R_3Si)_2NH$ $CF_3 - S - NH_2$ $(CF_3 - S)_2NH$ Pyridinium ion Quinolinium ion	88–92 97 133–136 82–90 67 81 99 90 96

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TABLE 6.57 Nitrogen-15 to Carbon-13 Spin Coupling Constants

Structure	J, Hz	Structure	J, Hz
Alkyl amines Cyclic alkyl amines Alkyl amines protonated Aryl amines Aryl amines protonated CH ₃ CO—NH ₂ H ₂ N—CO—NH ₂ Aryl—NO ₂	4-4.5 2-2.5 4-5 10-14 9 14-15 20 15	Alkyl $-NO_2$ R-CN $CH_3-N \equiv \bar{C}$ H_3C-N $-N \equiv C$ Diaryl azoxy anti syn	11 18 10 9 18 13

TABLE 6.58 Nitrogen-15 to Fluorine-19 Spin Coupling Constants

Structure	J, Hz	Structure	J, Hz
NF ₃	155	Pyridine	
F_4N_2	164	2-F	52
FNO ₂	158	3-F	4
F ₃ NO	190	2,6-di-F	37
F ₃ C—O—NF ₂	164–176	Pyridinium ion	
FCO—NF ₂	221	2-F	23
$(NF_4)^+SbF_6^-$	323	3-F	3
$(NF_4)^+ AsF_6^-$	328	Quinoline, 8-F	3
$(N_2F)^+AsF_6^-$	459	Aniline	
F ₃ C—NO ₂	215	2-F	0
-		3-F	0
F		4-F	1.5
$N=N$ $(^2J=10)$	190	Anilinium ion	
14=14		2-F	1.4
F		3-F	0.2
F F		4-F	0
$N = N$ $(^2J = 52)$		203	

TABLE 6.59 Fluorine-19 Chemical Shifts *Values given in ppm on the* δ *scale, relative to CCl*₃F

Substituent group	δ, ppm	Substituent group	δ, ppm
—SO ₂ —F	-67 to -42	R—CF ₂ Cl	61–71
	(aryl) (alkyl)	>C—CF ₃ and aryl—CF ₃	56–73
-CO-F	-29 to -20	-CS-CF ₃ >CF-CF ₃	70
>N-CO-F	-5		71–73
Aryl—CF ₂ Cl	49	$ \begin{array}{c c} -S - CF_3 \\ -S - CF_2 - S - \end{array} $	41
—CF ₂ I	56		39
-CF ₂ Br	63	>P—CF ₃	46–66

TABLE 6.59 Fluorine-19 Chemical Shifts (*continued*)

Substituent group	δ, ppm	Substituent group	δ , ppm
$>$ N $-$ CF $_3$	40–58	Perfluorocycloalkane	131–138
$>N-CF_2-C$	85-127	>CF-CF ₃	163-198
$-O-CF_2-R$	70-91	>CF(CF ₃) ₂	180-191
$-O-CF_2-CF_3$	70-91	—CFH—	198-231
$-CH_2-CF_3$	76–77	—CFH,	235-244
HO—CO—CF ₃	77	$F_2C = CF_2$	133
$-CHF-C\underline{F}_3$	81		
$-CF_2-C\underline{F}_3$	78–88	F_c CF_2-CF_2H	
—CS—F	81	C=C	
$CF_3-C-N \le$	84–96		
$-CO-CF_2-C\underline{F}_3$	83	\mathbf{F}_{t} \mathbf{F}_{g}	
$-CF_2-$	86-126	cis (Z)	108
$-CF_2Br$	91	trans (E)	92
$-C-CF_2-S-$	91–98	gem	192
-CF=	180-192		
$-C\underline{F}_2-CF_3$	111	F_2 F_3	
-CO-CF ₂ -	116–131	H	
$-C(halide)-CF_2-$	119–128	C=C H	
$-C\underline{F}_2-CF_3$	121–125		
$-CF_2-CF_2-$	121–129	H F ₁	
$-CF_2-CH_2-$	122–133	F-1	126
$-C\underline{F}_2-CHF_2$	128–132	F-2	155
$-CF_2H$	136–143	F-3	162
N		CI <u>F</u> C=CH-CF ₃	61
>F ₂	151–156	Cycloalkenes	
•		$=$ CF $-$ C \underline{F}_2 $-$	
\wedge		C(CF ₃ or H)—	101–113
$\langle \rangle F_2$	147	$-CF_2-C\underline{F}_2-$	
V		$C(CF_3 \text{ or } CH_3) =$	110–114
	06 122	$-CF_2-C\underline{F}_2-CH=$	113–116
$ \rangle F_2$	96–133	$-CF_2-C\underline{F}_2-CF=$	119–122
		Aryl—F	113
		C ₁₀ H ₇ —F F-1	127
F	150	F-1 F-2	127
\checkmark	159		114
Cyclohexane-F	210	C ₆ H ₅ —C ₆ H ₄ —F F-2	117
	(axial)	F-2 F-3	117
	to	F-3 F-4	109
	240	C_6F_6	163
	(equatorial)	C ₆ 1 6	103
	(equatorial)		

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TABLE 6.60 Fluorine-19 Chemical Shifts for Standards

Substance	Formula	δ, ppm
Trichlorofluoromethane	CFCl ₃	0.0
α, α, α -Trifluorotoluene	C ₆ H ₅ CF ₃	63.8
Trifluoroacetic acid	CF ₃ COOH	76.5
Carbon tetrafluoride	CF_4	76.7
Fluorobenzene	C_6H_5F	113.1
Perfluorocyclobutane	C_4F_8	138.0

TABLE 6.61 Fluorine-19 to Fluorine-19 Spin Coupling Constants

Structure	$J_{ m FF},{ m Hz}$
F ₂ C cycloalkane	212–260
Unsaturated compounds $\geq C = C \leq$	
gem	30–90
trans	115–130
cis	9–58
Aromatic compounds, monocyclic	
ortho	18–22
meta	0–7
para	12–15
Alkanes	
CFCl ₂ —CF ₂ —CFCl ₂	6
CFCl ₂ —CF ₂ —CCl ₃	5
CF ₂ Cl—CF ₂ —CF ₂ Cl	1
CF_3 — CF_2 — CF_2 Cl (or — CF_3)	<1
CF_3 — CF_2 — CF_2 Cl	2
CF_3 — CF_2 — CF_2 Cl	9
$CF_3 - CF_2 - CF_3$	7
-=32 -=3	· ·

TABLE 6.62 Silicon-29 Chemical Shifts

Values given in ppm on the δ scale relative to tetramethylsilane

	n					
Substituent group X in $(CH_3)_{4-n}SiX_n$	1	2	3	4		
—F	35	9	-52	-109		
−Cl −Br	30	32	13	-19		
—Br	26	20	-18	-94		
—I	9	-34	-18	-346		
—Н	-19	-42	-65	-93		
$-C_2H_5$	2	5	7	8		

TABLE 6.62 Silicon-29 Chemical Shifts (*continued*)

				n	
Substituent group X in $(CH_3)_{4-n}SiX_n$	1	2		3	4
$\begin{array}{l} -C_6H_5 \\ -CH = CH_2 \\ -Oalkyl \\ -Oaryl \\ -O-CO-alkyl \\ -N(CH_3)_2 \end{array}$	-5 -7 14-17 17 22 6	-3 to	-9 -14 -6 -6 4 -2	-12 -21 -41 to -45 -54 -43 -18	-23 -79 to -83 -101 -75 -28
Structure	δ, p	pm		Structure	δ, ppm
Hydrides H ₃ Si — —H ₂ Si — HSi ≦ Silicates Orthosilicate anions Silicon in end position Silicon in middle Branching silicons Cross-linked silicons Methyl siloxanes (CH ₃) ₂ Si — O — (end position O— (CH ₃) ₂ Si (middle) O— CH ₃ Si(H) (middle) O—	-39 to -5 to2 to69 to -77 to -85 to -93 to -107 to -18 to -35 to	-37 -39 -72 -81 -89 -97 0-120	Polys F ₃ S Cl ₃ (Cl (CH (CH	0-	-105 to -110

TABLE 6.63 Phosphorus-31 Chemical Shifts *Values given in ppm on the* δ *scale, relative to* 85% H_3PO_4

	Identical atoms attached directly	Non-ide	Non-identically substituted phosphorus			
Structure	to phosphorus	$R = CH_3$	$R = C_2H_5$	$R = C_6 H_5$		
P_4	461					
PR ₃		62	20	6		
PHR ₂		99	56	41		
PH_2R		164	128	122		
PH ₃	241					
PF ₃	-97					
PRF ₂			-168	-207		

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TABLE 6.63 Phosphorus-31 Chemical Shifts (*continued*)

	Identical atoms	Non-iden	tically substituted ph	osphorus
Structure	attached directly to phosphorus	$R = CH_3$	$R = C_2H_5$	$R = C_6 H_5$
PCl ₃ PRCl ₂ PR ₂ Cl PBr ₃ PRBr ₂ PR ₂ Br PI ₃ P(CN) ₃ P(SiR ₃) ₃ P(OR) ₂ Cl P(OR)Cl ₂ P(SR) ₃ P(SR) ₂ Cl P(SR) ₂ Cl P(SR) ₂ Br P(SR)Br ₂ P(NR ₂) ₃ P(NR ₂)Cl ₂ P(NR ₂) ₃ P(NR ₂)Cl ₂ PR ₂ (NR ₂) P ₂ P—PF ₂ Cl ₂ P—PCl ₂ I ₂ P—PCl ₂ I ₂ P—PL ₂ PH ₂ ⁻ K ⁺ P(CF ₃) ₃	-220 -227 -178 136 -136 -226 -155 -170 255 3	-192 -94 -184 -91 251 -141 -169 -114 -125 -188 -206 -204 -123 -166 -86 -39	-196 -119 -194 -116 -139 -165 -177 -115 -186 -211 -118 -162 -100 -62	-162 -81 -152 -71 -127 -157 -173 -132 -183 -204 -184 -151 -100
P ₄ O ₆	-113 Identical atoms	Non-ident	ically substituted pho	osphorus
Structure	attached directly to phosphorus	X = F	X = Cl	X = Br
P(NCO) ₃ P(NCO) ₂ X P(NCO)X ₂ P(NCS) ₃ P(NCS) ₂ X P(NCS)X ₂	-97 -86	-128 -131	-128 -166 -114 -155	-127 -112 -153
Structure	Identical atoms attached directly	Non-ident	ically substituted pho	osphorus
	to phosphorus	$R = CH_3$	$R = C_2H_5$	$R = C_6 H_5$
O=PR ₃ O=PHR ₂ O=PF ₃	36	-36 -63	-48	-25 -23

TABLE 6.63 Phosphorus-31 Chemical Shifts (*continued*)

	Identical atoms		Non-iden	tically substitut	ted pl	nosphorus
Structure	attached directly to phosphorus	R	= CH ₃	$R = C_2H_5$		$R = C_6 H_5$
O=PRF ₂	2	-	-27	-29		-11
$O = PCl_3$ $O = PRCl_2$	-2		-45	-53 -77		-34
$O = PR_2Cl$ $O = P(OR)_3$			-65 -1	1		-43 18
$O = P(OR)_2Cl$			-6	-3		6
$O = P(OR)Cl_2$ $O = PH(OR)_2$		_	−6 -19	-6 -15		-2
$O = PR_2(OC_2H_5)$			-50	-52		-31
$O = PR(OC_2H_5)_2$			-30	-33		-17
$O = P(NR_2)_3$ $O = PR_2(NR_2)$			-23 -44	-24		-2 -26
$O = P(OR)_2NH_2$			-15	-12		-3
$O = P(OR)_2(NCS)$				19		29
$O = P(SR)_3$ $O = PBr_3$	103	-	-66	-61		-55
$O = P(NCO)_3$	41					
$O = P(NCS)_3$	62					
$O = P(NH_2)_3$	-22					
	Identical ato					Identical atoms
Structure	attached director to phosphor		Struc	rtura		attached directly to phosphorus
Structure	to phosphol	us	Siruc	ture		to phosphorus
PF ₅	35		P			
PF ₆ ⁻ H ⁺	144 101		-O-P-	-O-		
PBr_5 $P(OC_2H_5)_5$	71		OI	R		
PO ₄ ³⁻	-6		(mid	dle group)		ca 18
$O = P[OSi(CH_3)_3]_3$	33		o			
H ₄ P ₂ O ₇ Phosphonates	11 -24 to -2		-O-P	-0-		
Phosphonium cation				O		
Alkyl	-43 to -32		O			
Aryl (O ₃ P—PO ₃) ⁴⁻	-35 to -18	3		(etc.) ich group)		ca 30
Polyphosphates	_9		(Drain	icii group)		Ca 50
O = P - O -						
(OR) ₂						
(end group	ca 6					

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TABLE 6.63 Phosphorus-31 Chemical Shifts (*continued*)

	Identical atoms	Non-identically substituted phosphorus			
Structure	attached directly to phosphorus	$R = CH_3$	$R = C_2H_5$	$R = C_6 H_5$	
$S = PR_3$		-59	-55	-43	
$S=PCl_3$	-29				
S=PRCl ₂		-80	-94	-75	
S=PR ₂ Cl		-87	-109	-80	
$S = PBr_3$	112				
$S = PRBr_2$		-21	-42	-20	
$S = PR_2Br$		-64	-98		
$S = P(OR)_3$		-73	-68	-53	
$S = P(OR)Cl_2$		-59	-56	-54	
$S = P(OR)_2CI$		-73	-68	-59	
$S = PH(OR)_2$		-74	-69	-59	
$S = P(SR)_3$		-98	-92	-92	
$S = P(NH_2)_3$	-60				
$S = P(NR_2)_3$		-82	-78		
$Se = P(OR)_3$		-78	-71	-58	
$Se = P(SR)_3$		-82	-76		
P(OR) ₅			71	86	
PRF ₄		30	30	42	
PR_2F_3		-9	-6		

TABLE 6.64 Phosphorus-31 Spin Coupling Constants

Substituent group	$J_{ m PH},{ m Hz}$	Substituent group	$J_{ m PH},{ m Hz}$
	180–225 134 160–210 1–6 14	>P-N-CH >P-C-CH P	8–25 0–4 7–10 2–4
α β γ (Halogen) ₂ P=CH \Rightarrow P-NH \Rightarrow P-O-CH ₃ \Rightarrow P-O-CH ₂ -R \Rightarrow P-O-CHR ₂ \Rightarrow P-SCH	12-22 30-40 14-20 16-20 10-28 11-15 6-10 3-7 5-20	$O = PHR_2$ $O = PH(S)R$ O_2PHR $O_2PH(N)$ $O_2PH(S \text{ or } Se)$ O_3PH $S(\text{ or } Se) = P - H$ $S(\text{ or } Se) = PHR_2$	210–500 490–540 500–575 560–630 630–655 630–760 490–650

TABLE 6.64 Phosphorus-31 Spin Coupling Constants

Substituent group	$J_{ m PH},{ m Hz}$	Substituent group	$J_{ m PH},{ m Hz}$
$O=P-CH_3$	7–15	p axial	600–860
		F equatorial	800-1000
O=P-CH=C	15–30	O = P - CF	110–113
O = P - CH - Aryl (or C=O)	15–30	O=P-F	980–1190
(Halogen) ₂ P—N—CH	9–18	P-O-P- <u>F</u>	2
1	11–15	Substituent group	$J_{\mathrm{PB}},\mathrm{Hz}$
S=P−CH >P−CH₃+	12–17	H_3B-P-N	80
≥P—H ⁺	490–600	j- j	
Substituent group	$J_{ m pp},{ m Hz}$	Substituent group	$J_{\mathrm{PP}},\mathrm{Hz}$
>P—F	1320–1420	>P-P<	220–400
RPF ₂	(1F) (3F) 1 140–1 290	O=P-P=O	330–500
R ₂ PF RP(N)F -O	1 020–1 110 920–985 (alkyl) (aryl)	S=P-P=S	15–500
PF -O	1 225–1 305	P-C-P	ca 70
(OCN)PF	1310	>P-O-P<	20–40
N-P		>P-S-P<	86–90
F	1 100–1 200	O = P - O = P = O	15–25
>P-CF	60–90	O=P-N=P=O H	8–30
P————F		P-N	5.66
ortho meta	0–60 1–7	$\stackrel{N}{\underset{P-N}{\bigvee}}$	5–66
para	0–3	P=N-P=N-	5–65

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ELECTRON SPIN RESONANCE

Electron paramagnetic resonance (EPR) is also referred to as electron spin resonance (ESR). In many respects, it is similar to NMR and the corresponding principles, discussed in the previous section, apply. The critical difference is that an unpaired electron spin is detected in this method instead of a nuclear spin. The method applies only to paramagnetic systems. The electron spin is more readily detected than is a nuclear spin and magnets on EPR instruments are correspondingly smaller and less expensive.

Certain transition metals such as cobalt (Co), copper (Cu), iron (Fe), manganese (Mn), nickel (Ni), and vanadium (V) have unpaired spins and are readily detectable by EPR. Likewise, organic radicals can be detected and studied. Numerous organic radicals have been studied by this method. When an unpaired electron spin is present, it will be observed at a characteristic resonance position. The resonance line is split by nuclei such as protons resulting in spin–spin coupling as observed in NMR. The coupling constant is referred to as "g" in EPR rather than "J" as in NMR. It is referred to as the hyperfine splitting or hyperfine coupling constant.

Certain radicals are especially stable and are of biological consequence or have been used as antioxidants. TEMPO radicals (TEMPO = 2,2,6,6-tetramethylpiperidin-1-oxyl) have been particularly well studied because they are readily prepared and extremely stable.

$$O_2N$$
 NO_2
 NO_2

A noticeable difference between NMR and EPR is that NMR is typically presented in absorption mode whereas EPR normally is presented in derivative mode. The EPR spectrum may be analyzed mathematically to determine the coupling pattern and thus the structural relationships. A database of software useful in EPR research is available at http://epr.niehs.nih.gov/software.html.

TABLE 6.65 Spin–Spin Coupling (Hyperfine Splitting Constants)

CH₃

0.6

Values of coupling constant a; given in gauss

Involves protons unless otherwise indicated.

mvorves protons	s uniess ouierwise maica	icu.	
H' Li 81	Na' K' 632 165	Cs. HĊ—H 3280 15	$H_2\dot{C}-H$ (¹ H) 22.8 (¹³ C) 41
$CH_3 - \dot{C} - H$ 26.8 22.3	CH ₃ -CH ₂ -30.3) ₂ —Ċ—H 4.7 21.2
$(CH_3)_3 - \dot{C}_{22.7}$	/ / \	16 CH ₂ =	$= CH - CH_2 - CH - H$ $= 28.5 \qquad 22.2$
$\dot{\triangle}$			
α 6.5β 23.4	α 21.3β 36.8γ 1.1	6.0	3.9
3.2	H−C≡C• 16.1	H 14.8 C C H 4.1 H ₂ C C H 4.1 H 13.9	ı
+	1.8	(+) (-) 6.5 3.J	2.9
(¹ H) 3.8 (¹³ C) 2.8	5.0	2.7 5.3	0.6 0.4 3.7
CH ₃ 0.8	CH ₃ 3.9	23	H ₂ —CH ₃
4.4			

CH₂-CH₃

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TABLE 6.65 Spin–Spin Coupling (Hyperfine Splitting Constants) (*continued*)

 TABLE 6.65
 Spin-Spin Coupling (Hyperfine Splitting Constants) (continued)

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TABLE 6.65 Spin–Spin Coupling (Hyperfine Splitting Constants) (continued)

IONIZATION POTENTIALS

The ionization potential is the energy required to remove an electron from an element or compound. Table 6.66A presents the ionization potentials for molecular species. The values are given in electron volts (eV). The values in parentheses are uncertainties in the final figure(s). Smaller numbers indicate lower energies or greater ease of electron removal. Table 6.66B is arranged alphabetically by element. Within an element, the compounds are arranged by increasing molecular weight.

TABLE 6.66A Ionization Potentials of Molecular Species

 $1\,eV = 23.061\,kcal\cdot mol^{-1}$ Values in parentheses are uncertainties in the final figure(s).

Carrier	Ionization potential, eV	Consider	Ionization potential,
Species	ev	Species	ev
Diborane(6)	12.0	2-Methyl-1-propene	9.23(2)
Pentaborane(9)	10.5	Cyclobutane	10.58
Hexaborane(10)	9.3(1)	Butane	10.63(3)
Trimethylborane	8.8(2)	Isobutane	10.57
Triethylborane	9.0(2)	Cyclopentadiene	8.97
Methane	12.6	1,2-Pentadiene	9.42
CD_4	12.888	1,3-Pentadiene	8.68
Acetylene	11.4	1,4-Pentadiene	9.58
C_2D_2	11.416(6)	2,3-Pentadiene	8.68
Ethylene	10.5	2-Methyl-1,4-butadiene	8.845(5)
Ethane	11.5	Cyclopentene	9.01(1)
Propyne	10.36	1-Pentene	9.50(2)
Allene	10.16(2)	cis-2-Pentene	9.11
Cyclopropene	9.95	trans-2-Pentene	9.06
Cyclopropane	10.09(2)	2-Methyl-1-butene	9.12(2)
Propane	11.1	3-Methyl-1-butane	9.51(3)
1,2-Butadiene	9.57(2)	3-Methyl-2-butene	8.69(2)
1,3-Butadiene	9.07	Cyclopentane	10.53(5)
1-Butyne	10.18(1)	Pentane	10.35
2-Butyne	9.9(1)	Isopentane	10.32
1-Butene	9.6	Neopentane	10.35

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TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
cis-2-Butene	9.13	Benzene	9.24
trans-2-Butene	9.13	Hexa-1,3-diene-5-yne	9.50
1,3-Hexadiyne	9.25	2,2,4-Trimethylpentane	9.86
1,4-Hexadiyne	9.75	2,2,3,3-Tetramethylbutane	9.79
1,5-Hexadiyne	10.35	Indene	8.81
2,4-Hexadiyne	9.75	β -Methylstyrene	8.35(1)
1-Methylcyclopentadiene	8.43(5)	Propylbenzene	8.72(1)
2-Methylcyclopentadiene	8.46(5)	Isopropylbenzene	8.69(1)
Cyclohexene	8.72	1,2,3-Trimethylbenzene	8.48
1-Hexene	9.45(2)	1,2,4-Trimethylbenzene	8.27
2,3-Dimethyl-2-butene	8.30	1,3,5-Trimethylbenzene	8.4
Cyclohexane	9.8	Naphthalene	8.12
Hexane	10.18	Azulene	7.42
2-Methylpentane	10.13	Butylbenzene	8.69(1)
3-Ethylbutane	10.08	sec-Butylbenzene	8.68(1)
2,2-Dimethylbutane	10.06	tert-Butylbenzene	8.68(1)
2,3-Dimethylbutane	10.00	1,2,3,5-Tetramethylbenzene	8.47(5)
Toluene	8.82(1)	1,2,4,5-Tetramethylbenzene	8.03
Cycloheptatriene	8.5	cis-Decalin	9.61(2)
Bicyclo[2.2.1]heptane	8.67	trans-Decalin	9.61(2)
Bicyclo[3.2.0]heptane	9.37	1-Methylnaphthalene	7.96(1)
1,2-Dimethylcyclopentadiene	8.1(1)	2-Methylnaphthalene	7.955(10)
5,5-Dimethylcyclopentadiene	8.22(5)	Pentamethylbenzene	7.933(10)
1,3-Cycloheptadiene	8.55	Hexamethylcyclopentadiene	7.74(5)
Norbornene	8.95(15)	Biphenyl	8.27(1)
4-Methylcyclohexene	8.91(1)	Hexamethylbenzene	7.85(2)
Methylcyclohexane	9.85(3)	Fluorene	8.63
Heptane	9.90(5)	Diphenylacetylene	8.85(5)
Phenylacetylene	8.815(5)	Anthracene	7.55
Styrene	8.47(2)	Phenanthrene	8.1
Cyclooctatetraene	8.0	1,2-Benzanthracene	8.01
Cubane	8.74(15)	1-Phenyldodecane	9.05(10)
Ethylbenzene	8.76(1)	3-Phenyldodecane	8.95(10)
o-Xylene	8.56	7-Phenyltridecane	8.91(10)
<i>m</i> -Xylene	8.58	1-Phenylicosane	9.34(10)
<i>p</i> -Xylene	8.44	2-Phenylicosane	9.22(10)
7-Methylcycloheptatriene	8.39(10)	3-Phenylicosane	8.95(10)
1-Methylspiroheptadiene	8.02(10)	4-Phenylicosane	9.01(10)
6-Methylspiroheptadiene	8.4(1)	5-Phenylicosane	9.04(10)
1,2,3-Trimethylcyclo-	0.4(1)	7-Phenylicosane	8.97(10)
pentadiene	7.96(5)	9-Phenylicosane	9.06(10)
1,5,5-Trimethylcyclo-	1.90(3)	N ₂	15.576
pentadiene	8.0(1)	NH ₃	10.2
4-Vinylcyclohexene	8.93(2)	NH ₃ N ₂ H ₂	9.85(10)
<i>cis</i> -1,2-Dimethylcyclohexane	1 ' '	2 2	
trans-1,2-Dimethylcyclo-	10.08(2)	N_2H_4 HCN	8.74(6) 13.8
hexane	10.08(3)		13.8
пелане	10.00(3)	C_2N_2	15.0

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 TABLE 6.66A
 Ionization Potentials of Molecular Species (continued)

Species	Ionization potential, eV	Species	Ionization potential, eV
Methylamine	8.97	<i>N,N</i> -Dimethyl- <i>p</i> -toluidine	7.33
Acetonitrile	12.2	Tripropylamine	7.23
Ethyleneimine	9.94(15)	N-Butylaniline	7.53
Ethylamine	8.86(2)	N,N-Diethylaniline	6.99
Dimethylamine	8.24(2)	<i>N,N</i> -Diethylaniline <i>N,N</i> -Dimethyl-4-ethylaniline	7.38
Acrylonitrile	* *	<i>N,N</i> -2,4-Tetramethylaniline	7.17
Propionitrile	10.91(1)	<i>N</i> , <i>N</i> -2,4-Tetramethylaniline	7.17
	11.84(2)		7.25
Propylamine	8.78(2)	N,N-3,5-Tetramethylaniline	
Isopropylamine	8.72(3)	N,N-Diethyl-4-toluidine	6.93
Trimethylamine	7.82(2)	N,N-Dimethyl-4-	7.41
3-Butenonitrile	10.39(1)	isopropylaniline	7.41
Pyrrole	8.20(1)	Diphenylamine	7.25(3)
Butyronitrile	11.67(5)	N,N-Dipropylaniline	6.96
Pyrrolidine	8.41	N,N-Dimethyl-4-tert-	5 .40
Butylamine	8.71(3)	butylaniline	7.43
sec-Butylamine	8.70	<i>N,N</i> -Dibutylaniline	6.95
Isobutylamine	8.70	Triphenylamine	6.86(3)
tert-Butylamine	8.64	Diazirine	10.18(5)
Diethylamine	8.01(1)	Diazomethane	8.999(1)
Pyridine	9.3	Methylhydrazine	8.00(6)
Aniline	7.7	1,1-Dimethylhydrazine	7.67(5)
2-Methylpyridine	9.02(3)	1,2-Dimethylhydrazine	7.75(10)
3-Methylpyridine	9.04(3)	o-Diazine	9.9
4-Methylpyridine	9.04(3)	<i>m</i> -Diazine	9.9
Cyclohexylamine	8.86	<i>p</i> -Diazine	9.8
Dipropylamine	7.84(2)	1,1-Diethylhydrazine	7.59(5)
Diisopropylamine	7.73(3)	1-Butyl-1-methylhydrazine	7.62(5)
Triethylamine	7.50(2)	<i>p</i> -Bis(dimethylamino)benzene	6.9
Benzonitrile	9.705(10)	Methyl azide	9.5(1)
N-Methylaniline	7.32	O_2	12.063(1)
<i>m</i> -Toluidine	7.50(2)	O_3	12.3(1)
2,3-Dimethylpyridine	8.85(2)	Water (and D ₂ O)	12.6
2,4-Dimethylpyridine	8.85(3)	H ₂ O ₂	11.0
2,6-Dimethylpyridine	8.85(2)	CO	14.013(4)
Phenylacetonitrile	9.4(5)	CO ₂	13.769(30)
3-Methylbenzonitrile	9.66(5)	NO	9.25
4-Methylbenzonitrile	9.76	N ₂ O	12.894
<i>N</i> -Ethylcyclohexylamine	7.56	NO ₂	9.79
<i>N,N</i> -Dimethylcyclo-		Formaldehyde	10.88
hexylamine	7.12	Methanol	10.84
Dibutylamine	7.69(3)	Acetaldehyde	10.2
N-Propylaniline	7.54	Ethylene oxide	10.6
<i>N</i> -Ethyl- <i>N</i> -methylaniline	7.37	Ethanol	10.49
<i>N</i> , <i>N</i> -Dimethyl- <i>o</i> -toluidine	7.37	Dimethyl ether	9.98
<i>N</i> , <i>N</i> -Dimethyl- <i>m</i> -toluidine	7.35	Propenal	10.10(1)
Propionaldehyde	9.98	Diphenyl ether	8.82(5)
1 Topionalucity uc	7.70	Diplicity retires	0.02(3)

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TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	potential, eV	Species	Ionization potential, eV
Acetone	9.69	Benzophenone	9.4
Allyl alcohol	9.67(5)	4-Methylbenzophenone	9.13(5)
Methyl vinyl ether	8.93(2)	Formic acid	11.05(1)
Propylene oxide	10.22(2)	Acetic acid	10.69(3)
Trimethylene oxide	9.667(5)	Methyl formate	10.815(5)
1-Propanol	10.1	Propionic acid	10.24(1)
2-Propanol	10.15	Ethyl formate	10.61(1)
Furan	8.89	Methyl acetate	10.27(2)
2-Butenal	9.73(1)	Dimethoxymethane	10.00(5)
Butyraldehyde	9.86(2)	Vinyl acetate	9.19(5)
2-Methylpropionaldehyde	9.74(3)	2,3-Butanedione	9.24(3)
2-Butanone	9.5	Butanoic acid	10.16(5)
Tetrahydrofuran	9.42	Isobutyric acid	10.02(5)
1-Butanol	10.04	Propyl formate	10.54(1)
Diethyl ether	9.6	Ethyl acetate	10.11(2)
Cyclopentanone	9.26(1)	Methyl propionate	10.15(3)
Dihydropyran	8.34(1)	1,4-Dioxane	9.13(3)
Pentanal	9.82(5)	1,1-Dimethoxyethane	9.65(3)
3-Methylbutyraldehyde	9.71(5)	2-Furaldehyde	9.21(1)
2-Pentanone	9.37(2)	2,4-Pentanedione	8.87(3)
3-Methyl-2-butanone	9.30(2)	Butyl formate	10.50(2)
3-Pentanone	9.32(1)	Isobutyl formate	10.46(2)
Cyclopentanone	9.25(1)	Propyl acetate	10.04(3)
Phenol	8.51	Isopropyl acetate	9.99(1)
4-Methyl-3-penten-2-one	9.08(3)	Ethyl propionate	10.00(2)
Cyclohexanone	9.14(1)	Methyl butyrate	10.07(3)
2-Hexanone	9.35	Methyl isobutyrate	9.98(2)
4-Methyl-2-pentanone	9.30	Diethoxymethane	9.70(5)
3,3-Dimethyl-2-butanone	9.17(3)	1,4-Quinone	9.67(2)
Dipropyl ether	9.27(5)	Butyl acetate	9.56(3)
Diisopropyl ether	9.20(5)	Isobutyl acetate	9.97
Benzaldehyde	9.52	sec-Butyl acetate	9.91(3)
Tropone	9.68(2)	Benzoic acid	9.73(9)
Benzyl alcohol	9.14(5)	p-Hydroxybenzaldehyde	9.32(2)
Methoxybenzene m-Cresol	8.21(2)	α-Hydroxyacetophenone Methyl benzoate	9.33(5)
	8.52(5) 9.33(3)	1	9.35(6)
2-Heptanone Acetophenone	9.33(3)	<i>p</i> -Methoxybenzaldehyde <i>m</i> -Hydroxyacetophenone	8.60(3) 8.67(5)
4-Methylbenzaldehyde	9.33(5)	<i>p</i> -Hydroxyacetophenone	8.70(3)
Benzyl methyl ether	8.85(3)	ρ -Hydroxyacetophenone α -Methoxyacetophenone	8.60(5)
Ethyl phenyl ether	8.13(2)	<i>m</i> -Methoxyacetophenone	8.53(5)
3-Methylanisole	8.31(5)	<i>p</i> -Methoxyacetophenone	8.62(5)
Propiophenone Propiophenone	9.27(5)	Methyl <i>p</i> -methylbenzoate	8.94(4)
3-Methylacetophenone	9.15(5)	<i>p</i> -Hydroxybenzophenone	8.59(5)
Phenyl benzoate	8.98(5)	N ₂ F ₄	12.04(10)
Benzil	8.78(5)	OF ₂	13.6
Methyl methoxyacetate	9.56(5)	XeF ₂	11.5(2)
Methyl <i>p</i> -methoxybenzoate	8.43(4)	Fluoromethane	12.85(1)

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 TABLE 6.66A
 Ionization Potentials of Molecular Species (continued)

Species	Ionization potential, eV	Species	Ionization potential, eV
Diphenyl carbonate	9.01(5)	Fluoroethylene	10.37
Acetamide	9.77(2)	Fluorobenzene	9.2
<i>N,N</i> -Dimethylformamide	9.12(2)	1,2-Difluorobenzene	9.31
<i>N</i> -Methylacetamide	8.90(2)	1,4-Difluorobenzene	9.15
NN-Dimethylacetamide	8.81(3)	Trifluoroethylene	10.14
<i>N,N</i> -Diethylformamide	8.89(2)	3,3,3-Trifluoro-1-propene	10.9
2-Pyridinecarboxaldehyde	9.75(5)	o-Fluorophenol	8.66(1)
4-Pyridinecarboxaldehyde	10.12(5)	PH ₃	9.98
<i>N,N</i> -Diethylacetamide	8.60(2)	PF ₃	9.71
Phenyl isocyanate	8.77(2)	Methylphosphine	9.72(15)
Benzamide	9.4(2)	Ethylphosphine	9.47(50)
<i>p</i> -Aminobenzaldehyde	8.25(2)	Trimethylphosphine	8.6(2)
<i>p</i> -Methoxyaniline	7.82	Triphenylphosphine	7.36(5)
Acetanilide	8.39(10)	S ₆	9.7
<i>m</i> -Aminoacetophenone	8.09(5)	S ₇	9.2(3)
<i>p</i> -Aminoacetophenone	8.17(2)	Hydrogen sulfide	10.4
α -Cyanoacetophenone	9.56(5)	Carbon disulfide	10.080
Nitromethane	11.1	Sulfur dioxide	12.34(2)
Nitroethane	10.88(5)	Methanethiol	9.440(5)
1-Nitropropane	10.81(3)	Ethylene sulfide	8.87(15)
2-Nitropropane	10.71(5)	Ethanethiol	9.285(5)
Nitrobenzene	9.92	Dimethyl sulfide	8.685(5)
<i>m</i> -Nitrotoluene	9.65(5)	Propylene sulfide	8.6(2)
<i>p</i> -Nitrotoluene	9.87	1-Propanethiol	9.195
o-Nitroaniline	8.66	Ethyl methyl sulfide	8.55(1)
<i>m</i> -Nitroaniline	8.7	Thiophene	8.860(5)
<i>p</i> -Nitroaniline	8.85	Methyl 1-propenyl sulfide	8.7(2)
Ethyl nitrate	11.22	1-Butanethiol	9.14(2)
Propyl nitrate	11.07(2)	Diethyl sulfide	8.430(5)
p-Nitrophenol	9.52	Methyl propyl sulfide	8.80(15)
<i>p</i> -Nitrobenzaldehyde	10.27(1)	Isopropyl methyl sulfide	8.7(2)
<i>m</i> -Nitroacetophenone	9.89(5)	Thiophenol	8.32(1)
<i>p</i> -Nitroacetophenone	10.07(2)	2-Ethylthiophene	8.8(2)
Methyl p-nitrobenzoate	10.20(3)	Dipropyl sulfide	8.5
F_2	15.7	Methyl phenyl sulfide	8.9
HF	15.77(2)	2-Propylthiophene	8.6(2)
BF ₃	15.5	2-Butylthiophene	8.5(2)
C_2F_4	10.12	Dimethyl disulfide	8.46(3)
Hexafluorobenzene	9.97	Diethyl disulfide	8.27(3)
trans-N ₂ F ₂	13.1(1)	COS	11.17(1)
NF ₃	13.2(2)	SO_2F_2	13.3(1)
Methyl isothiocyanate	9.25(3)	<i>p</i> -Dichlorobenzene	8.95
Methyl thiocyanate	10.065(10)	Chloroform	11.42(3)
Ethyl isothiocyanate	9.14(3)	Trichloroethylene	9.45
Ethyl thiocyanate	9.89(1)	1,1,2,2-Tetrachloroethane	11.10(5)
Phenyl isothiocyanate	8.520(5)	CNCI	12.49(4)
Tolyl thiocyanate	9.06(5)	CF ₃ Cl	12.91(3)
Thiourea	8.50(5)	Chlorotrifluoroethylene	10.4(2)

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
1-Methylthiourea	8.29(5)	Chloropentafluorobenzene	10.4(1)
1-Wedryttmodrea 1-Vinylthiourea	8.29(5)	Dichlorodifluoromethane	12.31(5)
1,1-Dimethylthiourea	8.34(5)	CF ₃ CCl=CClCF ₃	10.36(1)
1,3-Dimethylthiourea	8.17(5)	Trichlorofluoromethane	11.77(2)
1,1,3-Trimethylthiourea	7.93(5)	CF ₃ CCl ₃	11.78(3)
Tetramethylthiourea	7.95(5)	CFCl ₂ CF ₂ Cl	11.78(3)
CH ₃ COSH	10.00(2)	ClO ₃ F	13.6(2)
Cl ₂	11.48(1)	1-Bromo-1-propene	9.30(5)
HCl	12.74	1 1	
CCl ₄		1-Bromopropane	10.18(1)
7	11.47(1)	2-Bromopropane 1-Bromobutane	10.075(10)
Tetrachloroethylene	9.32(1)		10.125(10)
PCl ₃	9.91	2-Bromobutane	9.98(1)
Chloromethane Chloroethane	11.3 10.97	1-Bromo-2-methylpropane	10.09(2)
		2-Bromo-2-methylpropane	9.89(3)
Chloroethylene	9.996	1-Bromopentane	10.10(2)
1-Chloro-1-propyne	9.9(1)	Bromobenzene	8.98(2)
1-Chloropropane	10.82(3)	o-Bromotoluene	8.78(1)
2-Chloropropane	10.78(2)	<i>m</i> -Bromotoluene	8.81(2)
1-Chlorobutane	10.67(3)	p-Bromotoluene	8.67(2)
2-Chlorobutane	10.65(3)	Dibromomethane	10.49(2)
1-Chloro-2-methylpropane	10.66(3)	cis-1,2-Dibromoethylene	9.45
2-Chloro-2-methylpropane	10.61(3)	trans-1,2-Dibromoethylene	9.46
Chlorobenzene	9.07	1,1-Dibromoethane	10.19(3)
α-Chlorotoluene	9.19(5)	1,3-Dibromopropane	10.07(2)
o-Chlorotoluene	8.83(2)	Bromoform	10.51(2)
<i>m</i> -Chlorotoluene	8.83(2)	Tribromoethylene	9.27
<i>p</i> -Chlorotoluene	8.69(2)	Cyanogen bromide	11.95(8)
endo-5-Chloro-2-norbornene	9.10(15)	Bromotrifluoromethane	11.89
exo-5-Chloro-2-norbornene	9.15(15)	2-Bromopyridine	9.65(5)
Dichloromethane	11.35(2)	4-Bromopyridine	9.94(5)
cis-1,2-Dichloroethylene	9.65	Acetyl bromide	10.55(5)
trans-1,2-Dichloroethylene	9.64	Methyl bromoacetate	10.37(5)
1,2-Dichloroethane	11.12(5)	CF ₂ BrCH ₂ Br	10.83(1)
2,3-Dichloro-1-propene	9.82(3)	Bromochloromethane	10.77(1)
1,2-Dichloropropane	10.87(5)	1-Bromo-2-chloroethane	10.63(3)
1,3-Dichloropropane	10.85(5)	Bromodichloromethane	10.88(5)
o-Dichlorobenzene	9.06	Bromotrimethylsilane	10.24(2)
<i>m</i> -Dichlorobenzene	9.12(1)	I_2	9.28(2)
HI	10.39	CF ₃ CF ₂ CF ₂ CH ₂ Cl	11.84(2)
ICI	10.31(2)	Dichlorofluoromethane	12.39(20)
IBr	9.98(3)	Chlorotrimethylsilane	10.58(4)
Iodomethane	9.54	Trichloromethylsilane	11.36(3)
Iodoethane	9.33	Trichlorovinylsilane	10.79(2)
1-Iodopropane	9.26(1)	Trichloroethylsilane	10.74(4)
2-Iodopropane	9.17(2)	Trichloroisopropylsilane	10.28(10)
1-Iodobutane	9.21(1)	$C_2H_5V(CO)_4$	8.2(3)
2-Iodobutane	9.09(2)	Cr(CO) ₆	8.03(3)
1-Iodo-2-methylpropane	9.18(2)	$C_2H_5Mn(CO)_3$	8.3(4)

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 TABLE 6.66A
 Ionization Potentials of Molecular Species

Species	Ionization potential, eV	Species	Ionization potential, eV
2-Iodo-2-methylpropane	9.02(2)	Fe(CO) ₅	7.95(3)
1-Iodopentane	9.19(1)	Ni(CO) ₄	8.28(3)
Iodobenzene	8.73	Mo(CO) ₆	8.12(3)
o-Iodotoluene	8.62(1)	W(CO) ₆	8.18(3)
<i>m</i> -Iodotoluene	8.61(3)	As_4	9.07(7)
<i>p</i> -Iodotoluene	8.50(1)	Arsine	10.03
RuO ₄	12.33(23)	AsCl ₃	11.7(1)
2-Chloropyridine	9.91(5)	Trimethylarsine	8.3(1)
4-Chloropyridine	10.15(5)	Triphenylarsine	7.34(7)
Acetyl chloride	11.02(5)	Br ₂	10.54(3)
1-Chloro-2-propanone	9.99	HBr	11.62(3)
2-Chlorophenol	9.28	BrCl	11.1(2)
4-Chlorophenol	9.07	Bromomethane	10.53
Benzoyl chloride	9.70(1)	Bromoethylene	9.80
4-Chlorobenzaldehyde	9.61(1)	Bromoethane	10.29
α -Chloroacetophenone	9.5	1-Bromo-1-propyne	10.1(1)
<i>p</i> -Chloroacetophenone	9.47(5)	OsO ₄	12.97(12)
Methyl chloroacetate	10.53(5)	Dimethylmercury	9.0
4-Methoxybenzoyl chloride	8.87(5)	Diethylmercury	8.5(1)
4-Chlorobenzoyl chloride	9.58(3)	Diisopropylmercury	7.6(1)
cis-Chlorofluoroethylene	9.86	CH ₃ HgCl	11.5(2)
trans-Chlorofluoroethylene	9.87	Triphenylbismuth	7.3(1)
o-Chlorofluorobenzene	9.155(10)	Stibine	9.58
<i>m</i> -Chlorofluorobenzene	9.21(1)	Triphenylstibine	7.3(1)
<i>p</i> -Chlorofluorobenzene	9.43(2)	Tetramethylstannane	8.25(15)
Chlorodifluoromethane	12.45(5)	Tetramethylplumbane	8.0(4)
1-Chloro-1,1-difluoroethane	11.98(1)	Tetramethylgermane	9.2(2)

 TABLE 6.66B
 Alphabetical Listing of Ionization Potentials of Molecular Species

Species	IP (eV)	Species	IP (eV)
Acetylene	11.4	Butane	10.63(3)
Acetylene- d_2 ; C_2D_2	11.416	1-Butene	9.6
Allene	10.16	cis-2-Butene	9.13
Ammonia (NH ₃)	10.2	trans-2-Butene	9.13
Anthracene	7.55	1-Butyne	10.18(1)
Azine (N_2H_2)	9.85(10)	2-Butyne	9.9(1)
Azulene	7.42	Butylbenzene	8.69(1)
1,2-Benzanthracene	8.01	sec-Butylbenzene	8.68(1)
Benzene	9.24	tert-Butylbenzene	8.68(1)
Bicyclo[2.2.1]heptane	8.67	Carbon dioxide, CO ₂	12.888
Bicyclo[3.2.0]heptane	9.37	Cubane	8.74(15)
Biphenyl	8.27(1)	Cyclobutane	10.58
1,2-Butadiene	9.57(2)	1,3-Cycloheptadiene	8.55
1,3-Butadiene	9.07	Cycloheptatriene	8.5

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 TABLE 6.66B
 Alphabetical Listing of Ionization Potentials of Molecular Species (continued)

Species	IP (eV)	Species	IP (eV)	
Cyclohexane	9.8	4-Methylcyclohexene	8.91(1)	
Cyclohexene	8.72	1-Methylcyclopentadiene	8.43(5)	
Cyclooctatetraene	8	2-Methylcyclopentadiene	8.46(5)	
Cyclopentadiene	8.97	1-Methylnaphthalene	7.96(1)	
Cyclopentane	10.53(5)	2-Methylnaphthalene	7.955(10)	
Cyclopentene	9.01(1)	2-Methylpentane	10.12	
Cyclopropane	10.09	2-Methyl-l-propene	9.23(2)	
Cyclopropene	9.95	1-Methylspiroheptadiene	8.02(10)	
cis-Decalin	9.61(2)	6-Methylspiroheptadiene	8.4(1)	
trans-Decalin	9.61(2)	β-Methylstyrene	8.35(1)	
Diazomethane (C_2N_2)	13.6	Naphthalene	8.12	
Diborane	12	Neopentane	10.35	
2,2-Dimethylbutane	10.06	Nitrogen (N ₂)	15.576	
2,3-Dimethylbutane	10.02	Norbornene	8.95(15)	
2,3-Dimethyl-2-butene	8.3	Pentaborane(9)	10.5	
cis-1,2-Dimethylcyclohexane	10.08(2)	1,2-Pentadiene	9.42	
trans-1,2-Dimethylcyclohexane	10.08(3)	1,3-Pentadiene	8.68	
1,2-Dimethylcyclopentadiene	8.1(1)	1,4-Pentadiene	9.58	
5,5-Dimethylcyclopentadiene	8.22(5)	2,3-Pentadiene	8.68	
Diphenylacetylene	8.85(5)	Pentamethylbenzene	7.92(2)	
Ethane	11.5	Pentane	10.35	
Ethylbenzene	8.76(1)	1-Pentene	9.50(2)	
3-Ethylbutane	10.08	cis-2-Pentene	9.11	
Ethylene	10.5	trans-2-Pentene	9.06	
Fluorene	8.63	Phenanthrene	8.1	
Heptane	9.90(5)	Phenylacetylene	8.815(5)	
Hexaborane	9.3	1-Phenyldodecane	9.05(10)	
Hexa-1,3-diene-5-yne	9.5	3-Phenyldodecane	8.95(10)	
1,3-Hexadiyne	9.25	1-Phenylicosane	9.34(10)	
1,4-Hexadiyne	9.75	2-Phenylicosane	9.22(10)	
1,5-Hexadiyne	10.35	3-Phenylicosane	8.95(10)	
2,4-Hexadiyne	9.75	4-Phenylicosane	9.01(10)	
Hexamethylbenzene	7.85(2)	5-Phenylicosane	9.04(10)	
Hexamethylcyclopentadiene	7.74(5)	7-Phenylicosane	8.97(10)	
Hexane	10.18	9-Phenylicosane	9.06(10)	
1-Hexene	9.45(2)	7-Phenyltridecane	8.9100)	
Hydrazine (N ₂ H ₄)	8.74(6)	Propane	11.1	
Hydrocyanic acid (HCN)	13.8	Propylbenzene	8.72(1)	
Indene	8.81	Propyne	10.36	
Isobutane	10.57	Styrene	8.47(2)	
Isopentane	10.37	1,2,3,5-Tetramethylbenzene	8.47(2)	
Isopropylbenzene	8.69(1)	1,2,4,5-Tetramethylbenzene	8.03	
	* *			
Methane	12.6	2,2,3,3-Tetramethylbutane Toluene	9.79	
2-Methyl-1,4-butadiene	8.845(5)		8.82(1)	
3-Methyl-1-butane	9.51(3)	Triethylborane		
2-Methyl-1-butene	9.12(2)	1,2,3-Trimethylbenzene	8.48	
3-Methyl-2-butene	8.69(2)	1,2,4-Trimethylbenzene	8.27	
7-Methylcycloheptatriene	8.39(10)	1,3,5-Trimethylbenzene	8.4	
Methylcyclohexane	9.85(3)	Trimethylborane	8.8	

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TABLE 6.66B Alphabetical Listing of Ionization Potentials of Molecular Species (continued)

Species	IP (eV)	Species	IP (eV)
1,2,3-Trimethylcyclopentadiene 1,5,5-Trimethylcyclopentadiene 2,2,4-Trimethylpentane 4-Vinylcyclohexene	7.96(5) 8.0(1) 9.86 8.93(2)	<i>m</i> -Xylene <i>o</i> -Xylene <i>p</i> -Xylene	8.58 8.56 8.44

 TABLE 6.67
 Ionization potentials of radical species

 $1 \, eV = 23.061 \, kcal \cdot mol^{-1}$

Values in parentheses are uncertainties in the final figure(s).

	Ionization potential,		Ionization potential,
Species	eV	Species	eV
ВН	9.77(5)	tert-Pentyl	7.1(1)
BH_2	11.4(2)	Neopentyl	8.3(1)
BF	11.3	Benzyne	9.6
C_2	12.0(6)	Cyclohexyl	7.7
C_3	12.6	Benzyl	7.76(8)
CH	11.1(2)	Cycloheptatrienyl	6.24(1)
CH ₂	10.396(3)	1-Methylnaphthyl	7.35
CH ₃	9.83	2-Methylnaphthyl	7.56(5)
CD_3	9.832(2)	(CH ₃) ₂ CCN	9.15(10)
C_2H_3	9.4	m-Nitrobenzyl	8.56(10)
C_2H_5	8.4	ОН	13.17(10)
$HC \equiv CCH_2$	8.25	HO_2	11.53(2)
Allyl	8.15	СНО	9.8
Cyclopropyl	8.05	CH₃CO	10.3
C_3H_6	9.73	C ₆ H ₅ O	8.84
Propyl	8.1	CF ₂	11.8
Isopropyl	7.5	NF_2	11.9
C_4H_2	10.2(1)	CH ₂ F	9.35
C_4H_4	9.87	CHF ₂	9.45
Cyclobutyl	7.88(5)	HS	10.5(1)
$CH_3CH = CHCH_2$	7.71(5)	CH ₃ S	8.06(10)
$CH_2 = C(CH_3)CH_2$	8.03(5)	C ₆ H ₅ S	8.63(10)
Butyl	8.64(5)	CCl ₃	8.78(5)
sec-Butyl	7.93(5)	CH ₂ Cl	9.32
Isobutyl	8.35(5)	CHCl ₂	9.30
tert-Butyl	7.42(7)	NH_2	11.3
Cyclopentyl	7.79(2)		

X-RAY DIFFRACTION

The X-ray diffraction method utilizes a monochromatic beam of X-rays to which a solid material is exposed. The beam of radiation interacts with the solid, and is both reflected and diffracted. The reflection pattern is recorded by a detector system sensitive to the X-radiation. Until recently, this involved an intricate mechanical device whose complex

motion permitted X-rays to be recorded over a range of positions, as the detector position changed. Automated instruments using this technology are often referred to as "4-circle diffractometers," a term that refers to this complex detector motion. Newer X-ray instruments use charge coupled devices (CCDs) to simultaneously detect X-ray diffraction position and intensity over a much broader area. This enhanced detection technology reduces, often dramatically, the time required for data acquisition.

The Bragg equation describes the relationship between the impinging X-radiation, the diffraction angle, and the separation between lattice planes in the crystal under study. The Bragg equation is generally written as

$$\theta = \sin^{-1}(\lambda/2d)$$

where θ is the angle of the diffracted beam (usually called a reflection), λ is the wavelength of the incident X-ray beam, and d is the inter-planar spacing. From the diffraction pattern, both position and intensity, one can obtain structural information about the crystal under study.

Two types of X-ray studies are commonplace: X-ray powder analysis and crystal structure determination. Even in powders, the regular arrangement of atoms within the solid leads to characteristic diffraction patterns. X-ray powder patterns may therefore be used to characterize solids in much the same way that a UV or IR spectrum will give useful information but not necessarily a definitive structure.

The X-ray powder pattern obtained for the sodium salt of 2-propylpentanoic acid $(CH_3CH_2CH_2)_2CHCOO^-Na^+$ is shown in Figure 6.2. The X-ray powder pattern was detected over a range 2θ , in this case $2-40^\circ$ from the incident beam. This is a typical range although other ranges are used as well. The peak intensities are expressed in counts per second (cps) and may vary from experiment to experiment. However, the ratios of the peak heights are characteristic. Thus, X-ray powder patterns obtained from different samples of the same compound should give very similar, if not identical, patterns. Because the X-ray powder patterns are complex, the identity of two spectra suggests that the compounds producing them are also identical.

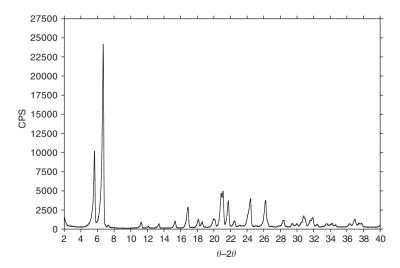


FIGURE 6.2 X-ray powder pattern of 2-propylpentanoic acid, (CH₃CH₂CH₂)₂CHCOO⁻Na⁺.

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The determination of a molecular structure from X-ray diffraction data is of critical importance to modern chemical and biological sciences. For small molecules, the structure is normally determined by direct methods. The X-ray diffraction pattern resulting from the interaction of X-rays with the electron clouds of different elements gives a pattern from which the elements present and their connectivity may be deduced. The expected diffraction pattern calculated for an apparent structure is then compared with the observed data to refine the result. Refinement factors (usually expressed as Rw) of 1–3% are common in modern small molecule structure determinations.

The Cambridge Structural Database is a repository for more than 250 000 (as of 2002) small molecule crystal structures. It is accessible at http://www.ccdc.cam.ac.uk/bysubscription.

The process is more complex for such large molecules as proteins. Typically, a model of the amino acid backbone will be constructed first to obtain a general sense of the overall structure. Amino acid sidechains will then be added and the experimental data are again compared with the calculated diffraction pattern. This process is repeated until the complete structure is obtained. Because the uncertainties are larger in these systems, the resolution of the structure is typically reported in Ångstroms. Structures that have a resolution of 3 Å can and do give important information, especially when the gross structure of a protein was previously unknown. Recent improvements in chemical and biological techniques, computers, and X-ray instrumentation (especially in detectors) have made resolutions in the 1–2 Å range more common.

A database, called the Protein Data Bank or "PDB," is a repository for protein structures. The database may be consulted at no charge and gives access to structures obtained by X-ray methods as well as by NMR and theoretical techniques. The Internet address is http://www.rcsb.org/pdb.

SECTION 7

PHYSICOCHEMICAL RELATIONSHIPS

LINEAR FRE	E ENERGY RELATIONSHIPS	7.2
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7.2 SECTION 7

LINEAR FREE ENERGY RELATIONSHIPS

Organic chemists have studied the influence of substituents on various reactions for the better part of a century. Linear free energy relationships have played an important role in this pursuit by correlating equilibrium and rate processes. One of the earliest examples is now known as the Hammett equation. It emerged from the observation that the acidities of benzoic acids correlated with the rates at which ethyl esters of benzoic acids hydrolyzed. The relationship was expressed as follows in which K represents an equilibrium constant and k is a rate constant. The proportionality constant, m, is the slope of the log–log data plot for the two processes.

$$m\log\frac{K}{K_0} = \log\frac{k}{k_0}$$

When ΔH and ΔS vary linearly for two processes or when ΔH or ΔS is constant, the free energy relationship will be linear. The common form of the relationship is either

$$\log \frac{K}{K_0} = \sigma \rho$$
 or $\log \frac{k}{k_0} = \sigma \rho$

for equilibrium or rate processes, respectively. The Greek letters rho (ρ) and sigma (σ) symbolize the reaction and substituent constants, respectively. These equations may be used to describe and understand the influence of substituents on a reaction. Separate sigma values are defined by this reaction for *meta* and *para* substituents and provide a measure of the total electronic influence (polar, inductive, and resonance effects) in the absence of conjugation effects. The correlation is not as useful for *ortho*-substituted aromatic compounds because steric or other proximity effects intercede.

Typically in aromatic systems, the inductive effect is transmitted about equally to the *meta* and *para* positions. Consequently, σ_m is an approximate measure of a substituent's inductive effect whereas σ_p gives an approximate measure of a substituent's resonance effect. Consider the dissociation of benzoic acids in water. This process is assigned a reaction constant ρ of 1. The reaction is illustrated using "Sub" to represent a substituent.

We may compare three *para*-substituted benzoic acids. The reference point is *para*-hydrogen, which has a σ_p constant of 0, by definition. The methoxy group is electron donating and has a σ_p constant of -0.27. Adding electrons to the benzoate anion (structure at right, above) should make the anion less stable. Thus, the ability to dissociate a cation (the acidity) should be diminished. The pK_A is $-\log K_A$ so the higher the pK_A, the lower the acidity (the weaker the acid). In contrast, the nitro group is electron withdrawing. Its σ_p constant is +0.78 and its presence in the benzoate anion should be stabilizing. A more stable conjugate base implies a stronger acid and, indeed, the pK_A for 4-nitrobenzoic acid is 3.44. Because these values are logarithmic, there is an order of magnitude difference in the acidities as a result of these substituents.

Comparison of acidities and sigma constants for three benzoic acids

Compound	соон	COOH	COOH NO ₂
Substituent σ_p pK_A	OCH ₃	H	NO ₂
	-0.27	0.00	0.78
	4.49	4.20	3.44

Values of Hammett sigma constants are listed in Table 7.1. Taft sigma* (σ *) values may be used similarly with respect to aliphatic and alicyclic systems. Values of σ * constants are also listed in Table 7.1.

The reaction constant ρ is related to the reaction process rather than to the substituents present. A somewhat oversimplified way of considering ρ is to say that it indicates the demand the process makes on the substituents. The acidity of a benzoic acid, C_6H_3COOH , derivative is affected directly by substituents in the aromatic ring. Substituents exert somewhat less influence in phenylacetic acids, $C_6H_5CH_2COOH$, because the methylene group between carboxylate and the aromatic ring tends to insulate the latter from the former. This "insulation" is even greater for phenyipropanoic acids, $C_6H_5CH_2COOH$. The reaction constant ρ for dissociation of benzoic acid in water is set at 1.0. The reaction constants for dissociation of phenylacetic and phenylpropanoic acids are 0.49 and 0.21, respectively, under the same conditions. Values of the reaction parameter for some aromatic and aliphatic systems are given in Tables 7.2 and 7.3.

Since substituent effects in aliphatic systems and in *meta* positions in aromatic systems are essentially inductive in character, σ^* and σ_m values are related by the expression $\sigma_m = 0.217\sigma^* - 0.106$. Substituent effects fall off with increasing distance from the reaction center. The decline is generally a factor of 0.36 for the interposition of a —CH₂— group. This enables σ^* values to be estimated for R—CH₂— groups not otherwise available.

Modified sigma constants have been formulated for situations in which the substituent enters into resonance with the reaction center in an electron-demanding transition state (σ^+) or for an electron-rich transition state (σ^-) . Generally, σ^- constants give better correlations in reactions involving phenols, anilines, pyridines, and in nucleophilic substitutions. Values for some modified sigma constants are given in Table 7.4.

TABLE 7.1 Hammett and Taft Substituent Constants

	Hammett o	Hammett constants		
Substituent	$\sigma_{\scriptscriptstyle m}$	σ_p	Taft constant σ*	
—AsO ₃ H	-0.09	-0.02	0.06	
$-B(OH)_2$	0.01	0.45		
—Br	0.39	0.23	2.84	
—CH₂Br			1.00	
m -Br $\widetilde{\mathrm{C}_6}\mathrm{H}_4$ —		0.09		

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TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)

	Hammett constants		- Taft	
Substituent	$\sigma_{\scriptscriptstyle m}$	σ_p	constant σ^*	
o-BrC ₆ H ₄ —		0.08		
-CH ₃	-0.07	-0.17	0.0	
-CH ₂ CH ₃	-0.07	-0.15	-0.10	
-CH ₂ CH ₂ CH ₃	-0.05	-0.15	-0.12	
-CH(CH ₃) ₂ (isopropyl)	-0.07	-0.15	-0.19	
-CH ₂ CH ₂ CH ₂ CH ₃	-0.07	-0.16	-0.13	
-CH ₂ CH(CH ₃) ₂ (isobutyl)	-0.07	-0.12	-0.13	
-CH(CH ₃)CH ₂ CH ₃ (sec-butyl)		-0.12	-0.19	
$-C(CH_3)_3$ (t-butyl)	-0.10	-0.20	-0.30	
-CH ₂ CH ₂ CH ₂ CH ₃ (<i>n</i> -pentyl)	0.10	0.20	-0.25	
-CH ₂ CH ₂ CH(CH ₃) ₂ (isopentyl)			-0.17	
$-\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 \text{ (isopenty)}$ $-\text{CH}_2\text{C}(\text{CH}_3)_3 \text{ (}t\text{-amyl)}$		-0.23	-0.12	
2 1 3 3 1 • 1		-0.23		
-CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	0.07	0.21	-0.37	
-CH(CH ₂) ₂ (cyclopropyl)	-0.07	-0.21	0.15	
-CH(CH ₂) ₅ (cyclohexyl)		0.26	-0.15	
Υ		-0.26		
<u>~</u>				
\bigcup		-0.48		
~				
	0.06	0.04		
	0.06	0.04	0.56	
-CH=CH ₂ (vinyl, ethenyl)	0.02		0.56	
$-CH = C(CH_3)_2$			0.19	
$-CH = CHCH_3$, trans			0.36	
$-CH_2CH = CH_2$			0.0	
$-CH = CHC_6H_5$	0.14	-0.05	0.41	
-C≡CH	0.21	0.23	2.18	
$-C \equiv CC_6H_5$	0.14	0.16	1.35	
-CH ₂ C≡CH			0.81	
$-C_6H_5$ (phenyl)	0.06	-0.01	0.60	
$-CH_3C_6H_4$ (p -tolyl)		-0.5		
(1-naphthyl)			0.75	
$\Upsilon\Upsilon$				
(2-naphthyl)			0.75	
$-CH_2C_6H_5$ (benzyl)		0.46	0.22	
$-CH_2CH_2C_6H_5$ (2-phenylethyl)			-0.06	
$-CH(CH_3)C_6H_5$ (α -phenylethyl)			0.37	
$-CH(C_6H_5)_2$ (benzhydryl)			0.41	
H ₂			0.44	
``				
$\tilde{\Lambda}$ $\tilde{}$				
(2-furoyl)			0.25	
, L.»			-0.06	

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)

	Hammet	Taft	
Substituent	$\sigma_{\scriptscriptstyle m}$	σ_p	constant σ*
(2-thienyl)			1.31
S (2-mienyi)			0.21
CH ₂ — (2-thienylmethylene)			0.31
—CHO (formyl)	0.36	0.22	
—COCH ₃ (acetyl)	0.38	0.50	1.65
—COCH ₂ CH ₃ (propionyl)		0.48	
—COCH(CH ₃) ₂		0.47	
—COC(CH ₃) ₃		0.32	
—COCF ₃ (trifluoroacetyl)	0.65		3.7
—COC ₆ H ₅ (benzoyl)	0.34	0.46	2.2
—CONH ₂	0.28	0.36	1.68
−CONHC ₆ H ₅			1.56
-CH ₂ COCH ₃ (acetonyl)			0.60
-CH ₂ CONH ₂ (acetamido)			0.31
-CH ₂ CH ₂ CONH ₂			0.19
-CH ₂ CH ₂ CONH ₂			0.12
−CH ₂ CONHC ₆ H ₅			0.0
—COO ⁻ (carboxylate)	-0.1	0.0	-1.06
—COOH (carboxyl)	0.36	0.43	2.08
—CO—OCH ₃ (carbomethoxy)	0.32	0.39	2.00
—CO—OCH ₂ CH ₃ (carbethoxy)	0.37	0.45	2.12
-CH ₂ CO-OCH ₃			1.06
-CH ₂ CO-OCH ₂ CH ₃			0.82
−CH ₂ COOH			-0.06
—CH ₂ CH ₂ COOH	-0.03	-0.07	
—Cl	0.37	0.23	2.96
—CCl ₃ (trichloromethyl)	0.47		2.65
—CHCl ₂ (dichloromethyl)			1.94
—CH ₂ Cl (chloromethyl)	0.12	0.18	1.05
—CH ₂ CH ₂ Cl			0.38
-CH ₂ CCl ₃			0.75
-CH ₂ CH ₂ CCl ₃			0.25
-CH=CCl ₂			1.00
-CH ₂ CH=CCl ₂			0.19
p-ClC ₆ H ₄ — (p -chlorophenyl)		0.08	
—F	0.34	0.06	3.21
—CF ₃ (trifluoromethyl)	0.43	0.54	2.61
—CHF ₂ (difluoromethyl)			2.05
-CH ₂ F (fluoromethyl)			1.10
-CH ₂ CF ₃			0.90
-CH ₂ CF ₂ CF ₂ CF ₃			0.87
-C ₆ F ₅ (pentafluorophenyl)	-0.12	-0.03	
—Ge(CH ₃) ₃ (trimethylgermyl)		0.0	
—Ge(CH ₂ CH ₃) ₃ (triethylgermyl)		0.0	
—H	0.00	0.00	0.49
—I	0.35	0.28	2.46
—CH ₂ I (iodomethyl)			0.85
-N ₂ ⁺ (diazonio)	1.76	1.91	

7.6 SECTION 7

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)

	Hammett o	constants	- Taft
Substituent	$\sigma_{\scriptscriptstyle m}$	σ_p	constant σ*
-N ₃ (azido)	0.33	0.08	2.62
-NH ₂ (amino)	-0.16	-0.66	0.62
-NH ₃ +	1.13	1.70	3.76
-CH ₂ -NH ₂ (aminomethyl)			0.50
$-CH_2-NH_3^+$			2.24
-NH-CH ₃ (methylamino)	-0.30	-0.84	
$-NH-C_2H_5$ (ethylamino)	-0.24	-0.61	
$-NH-C_4H_9$ (butylamino)	-0.34	-0.51	
-NH(CH ₃) ₂ ⁺	0.5	0.01	4.36
$-NH_{\uparrow}^{+}$ $-CH_{3}$	0.96		3.74
$-NH_{2}^{+}$ $-C_{2}H_{5}$	0.96		3.74
$-N(CH_3)_3^+$ (trimethylammonium)	0.88	0.82	4.55
-N(CH ₃) ₂ (dimethylamino)	-0.2	-0.83	0.32
$-CH_2-N(CH_3)_3^+$	0.2	0.03	1.90
$-N(CF_3)_2$ [bis(trifluoromethyl)amino]	0.45	0.53	1.50
$p-H_2N-C_6H_5-(p-aminophenyl)$	0.43	-0.30	
-NH—CO—CH ₃	0.21	0.00	1.40
$-NH-CO-C_2H_5$	0.21	0.00	1.56
$-NH-CO-C_6H_5$	0.22	0.08	1.68
-NH-CHO	0.25	0.00	1.62
-NH-CO-NH ₂	0.23		1.31
-NH-OH (hydroxylamino)	-0.04	-0.34	1.31
-NH-CO-OC ₂ H ₅	0.33	0.54	1.99
-NH $-CO$ $-OC2H5 -CH2-NH-CO-CH3$	0.55		0.43
-CH2-NH-CO-CH3 $-NH-SO2-C6H5$			1.99
$-NH-NH_2$ (hydrazido)	-0.02	-0.55	1.99
$-NH-NH_2$ (hydrazido) $-C \equiv N$ (cyano)	0.56	0.66	3.30
	0.30		1.30
—CH₂—CN (cyanomethyl) —N≡O (nitroso)	0.17	0.01 0.12	1.30
$-NO_0$ (nitro)	0.71	0.12	4.0
= 1 /	0.71	0.76	
CH ₂ NO ₂ (nitromethyl) CH ₂ CH ₂ NO ₂ (2-nitroethyl)			1.40 0.50
$-CH_2$ $-CH_2$ $-NO_2$ (2-introethyl) $-CH$ $-CHNO_2$ (2-nitroethylenyl)	0.33	0.26	0.30
	0.55	0.20	
$m \cdot O_2N - C_6H_4 - (m \cdot \text{nitrophenyl})$		0.18	
p-O ₂ N—C ₆ H ₄ — (p -nitrophenyl)		0.24	
0211	0.43	0.41	
NO ₂ (picryl)	0.43	0.41	1 27
-N CO-CH ₃			1.37
CO-C ₆ H ₅			1.65
CO-CH ₃			
—O ⁻	-0.71	-0.52	
—OH (hydroxy)	0.12	-0.32	1.34
-O-CH ₃ (methoxy)	0.12	-0.27	1.81
-O-CI3 (inclinoxy) -O-C2H5 (ethoxy)	0.12	-0.24	1.68
	0.10	0.24	1.00

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)

	Hammett constants		Taft
Substituent	σμ	σр	constant σ*
$-O-C_3H_7$ (propoxy)	0.00	-0.25	1.68
—O—CH(CH ₃) ₂ (isopropoxy)	0.05	-0.45	1.62
$-O-C_4H_9$ (butoxy)	-0.05	-0.32	1.68
$-O-C_5H_9$ (cyclopentyloxy)			1.62
$-O-C_6H_{11}$ (cyclohexyloxy)	0.29		1.81
$-O-CH_2-C_6H_{11}$ (cyclohexylmethoxy)	0.18		1.31
$-O-C_6H_5$ (phenoxy)	0.25	-0.32	2.43
$-O-CH_2-C_6H_5$ (phenylmethoxy)		-0.42	
—OCF ₃ (trifluoromethoxy)	0.40	0.35	
P	00		
(3,4- methylenedioxyphenyl,		-0.27	
piperonyl)			
~°~~			
(3,4-ethylenedioxyphenyl)		0.12	
	0.39	-0.12	
-O-CO-CH ₃ (acetoxy)	0.39	0.31	3.86
-ONO ₂ (nitrate ester)			
$-O-N=C(CH_3)_2$			1.81
-ONH ₃			2.92
-CH ₂ -O ⁻	0.00	0.00	0.27
-CH ₂ -OH	0.08	0.08	0.31
-CH ₂ -O-CH ₃			0.52
-CH(OH)-CH ₃			0.12
-CH(OH)-C ₆ H ₅		0.24	0.50
p-HO—C ₆ H ₄ — (p-hydroxyphenyl)		-0.24	
$p\text{-CH}_3\text{O}$ — C_6H_4 — ($p\text{-methoxyphenyl}$)		-0.10	0.06
-CH ₂ -CH(OH)-CH ₃			-0.06
$-CH_2-C(OH)(CH_3)_2$	0.1	0.05	-0.25
-P(CH ₃) ₂ (dimethylphosphino)	0.1	0.05	
-P(CH ₃) ₃ (trimethylphosphino)	0.8	0.9	
$-P(CF_3)_2$	0.6	0.7	
—PO₃H [⊖]	0.2	0.26	
$-PO(OC_2H_5)_2$	0.55	0.60	1.00
—SH (thio, mercapto)	0.25	0.15	1.68
—SCH ₃ (methylthio)	0.15	0.00	1.56
$-S(CH_3)_2^+$ (dimethylsulfonium)	1.0	0.9	
—SCH ₂ CH ₃ (ethylthio)	0.23	0.03	1.56
—SCH ₂ CH ₂ CH ₃ (propylthio)			1.49
—SCH ₂ CH ₂ CH ₂ CH ₃ (butylthio)			1.44
—SC ₆ H ₁₁ (cyclohexylthio)			1.93
—SC ₆ H ₅ (phenylthio)	0.30		1.87
$-SC(C_6H_5)_3$ (triphenylmethylthio)			0.69
$-SCH_2C_6H_5$ (benzylthio)			1.56
$-SCH_2CH_2C_6H_5$ (phenethylthio)			1.44
—CH ₂ SH (thiomethyl)	0.03		0.62
-CH2SCH2C6H5			0.37
—SCF ₃ (trifluoromethylthio)	0.40	0.50	
—SCN (thiocyanato)	0.63	0.52	3.43

7.8 SECTION 7

TABLE 7.1 Hammett and Taft Substituent Constants (continued)

	Hammett o	constants	Taft
Substituent	σμ	σр	constant σ*
-S-CO-CH ₃	0.39	0.44	
$-S-CO-NH_2$	0.34		2.07
—SO—CH ₃ (methylsulfoxy)	0.52	0.49	
$-SO-C_6H_5$ (phenylsulfoxy)			3.24
$-CH_2-SO-CH_3$			1.33
—SO ₂ —CH ₃ (methylsulfonyl)	0.60	0.68	3.68
—SO ₂ —CH ₂ CH ₃ (ethylsulfonyl)			3.74
—SO ₂ —CH ₂ CH ₂ CH ₃ (propylsulfonyl)			3.68
$-SO_2-C_6H_5$ (phenylsulfonyl)	0.67		3.55
—SO ₂ —CF ₃ (trifluoromethylsulfonyl)	0.79	0.93	
$-SO_2-NH_2$	0.46	0.57	
$-CH_2-SO_2-CH_3$			1.38
$-SO_3^-$	0.05	0.09	0.81
−SO ₃ H		0.50	
—SeCH ₃	0.1	0.0	
—Se—C ₆ H ₁₁ (cyclohexylselenyl)			2.37
—SeCN	0.67	0.66	3.61
$-Si(CH_3)_3$	-0.04	-0.07	-0.81
-Si(CH ₂ CH ₃) ₃		0.0	
$-Si(CH_3)_2C_6H_5$			-0.87
$-Si(CH_3)_2$ $-O-Si(CH_3)_3$			-0.81
-CH2Si(CH3)3	-0.16	-0.22	-0.25
-CH ₂ CH ₂ Si(CH ₃) ₃			-0.25
$-Sn(CH_3)_3$		0.0	
-Sn(CH ₂ CH ₃) ₃		0.0	

TABLE 7.2 pK_A and Rho (ρ) Values for the Hammett Equation

pK_A	ρ
	1.05
8.49	0.87
9.70	2.15
1.84	0.76
6.97	0.95
10.70	0.86
4.78	1.03
10.00	1.06
8.31	1.16
	3.54 8.49 9.70 1.84 6.97 10.70 4.78 10.00

TABLE 7.2 pK_A and Rho (ρ) Values for the Hammett Equation (*continued*)

Acid	pK_A	ρ
C_6H_5 — SO_2 — NH — C_6H_4 — Y	8.31	1.74
Ar— CO — OH (benzoic acids)	4.21	1.00
$\overset{Y}{\longleftarrow} \overset{H}{\vdash} \overset{C}{\vdash} \overset{C}{\vdash} \overset{C}{\vdash} \overset{COOH}{\vdash} \text{(cinnamic acids)}$	4.45	0.47
Ar—OH (phenols)	9.92	2.23
CH2COOH (phenylacetic acids)	4.30	0.49
Y C≡c−cooH (phenylpropiolic acids, in aqueous 35% dioxane)	3.24	0.81
(CH₂)₂COOH		
(phenylpropionic acids)	4.45	0.21
Ar—CHOH—CF ₃ (phenyltrifluoromethylcarbinols)	11.90	1.01
N+-O- (pyridine-1-oxides, pyridine-N-oxides)	0.94	2.09
Y (2-pyridones, 2-hydroxypyridines)	11.65	4.28
HO (4-pyridones, 4-hydroxypyridines)	11.12	4.28
Y NH (pyrroles)	17.00	4.28
Y N COOH (5-substituted pyrrole-2-carboxylic acids)	2.82	1.40
Ar—CO—SH (thiobenzoic acids) Ar—SH (thiophenols)	2.61 6.50	1.0 2.2
Y CF ₃ (trifluoroacetophenone hydrates)	10.00	1.11
OH (5-substituted tropolones)	6.42	3.10
Cations resulting from protonation of		
Ar—CO—CH ₃ (acetophenones) Ar—NH ₂ (anilines)	-6.0 4.60	2.6 2.90
Y C-aryl-N,N'-dibutylamidines, in aqueous 50% ethanol)	11.14	1.41
N,N-Dimethylanilines	5.07	3.46
(isoquinolines)	5.32	5.90
1-Naphthylamines	3.85	2.81
2-Naphthylamines	4.29	2.81
Pyridines	5.18	5.90
(quinolines)	4.88	5.90

7.10 SECTION 7

TABLE 7.3 pK_A and Rho (ρ) Values for the Taft Equation

Acid	pK_A	Rho (ρ)
RCOOH	4.66	1.62
RCH ₂ COOH	4.76	0.67
RC≡C—COOH	2.39	1.89
$H_2C = C(R) - COOH$	4.39	0.64
$(CH_3)_2C = C(R) - COOH$	4.65	0.47
$Z-C_6H_5$ — CH = $C(R)$ — $COOH$	3.77	0.63
E - C_6H_5 — CH = $C(R)$ — $COOH$	4.61	0.47
R—CO—CH ₂ —COOH	4.12	0.43
HO—N=CR—COOH	4.84	0.34
RCH ₂ OH	15.9	1.42
RCH(OH) ₂	14.4	1.42
R¹CO—NHR²	22.0	3.1*
$CH_3CO-CR=C(OH)CH_3$	9.25	1.78
CH ₃ CO—CHR—CO—OC ₂ H ₅	12.59	3.44
R—CO—NHOH	9.48	0.98
$R^1R^2C = N - OH(R^1, R^2 \text{ are not acyl groups})$	12.35	1.18
HONN RCCCCH3	9.00	0.94
RCH(NO ₂) ₂	5.24	3.60
RSH	10.22	3.50
RCH ₂ SH	10.54	1.47
R—CO—SH	3.52	1.62
Cations resulting from protonation of		
RNH_2	10.15	3.14
R^1R^2NH	10.59	3.23
$R^1R^2R^3N$	9.61	3.30
$R^{1}R^{2}PH$	3.59	2.61
$R^1R^2R^3P$	7.85	2.67

 $^{*\}sigma*$ for R¹CO and R²

 TABLE 7.4
 Special Hammett Sigma Constants

Substituent	$\sigma_{_m}{^+}$	$\sigma_{\!p}^{\;+}$	σ_p^{-}
—CH ₃	-0.07	-0.31	-0.17
—C(CH ₃) ₃	-0.06	-0.26	
-C ₆ H ₅ -CF ₃ -F -Cl	0.11	-0.18	
—CF ₃	0.52	0.61	0.74
—F	0.35	-0.07	0.02
—Cl	0.40	0.11	0.23
—Br	0.41	0.15	0.26
—I	0.36	0.14	
$-c \equiv N$	0.56	0.66	0.88
-CH=O			1.13

TABLE 7.4 Special Hammett Sigma Constants (*continued*)

Substituent	$\sigma_{\scriptscriptstyle m}^{^+}$	$\sigma_p^{\;+}$	$\sigma_{p}^{\;-}$
-CO-NH ₂			0.63
—CO—CH ₃			0.85
—СООН	0.32	0.42	0.73
—CO—OCH ₃	0.37	0.49	0.66
—CO—OCH₂CH₃	0.37	0.48	0.68
-N ₂ ⁺			3.2
—NH ₂	0.16	-1.3	-0.66
$-N(CH_3)_2$		-1.7	
$-N(CH_3)_3^+$	0.36	0.41	
-NH-CO-CH ₃		-0.60	
-NO ₂	0.67	0.79	1.25
—OH		-0.92	
- 0 ⁻			-0.81
—OCH ₃	0.05	-0.78	-0.27
—SF ₅			0.70
—SCF ₃			0.57
-SO ₂ CH ₃			1.05
$-SO_2^2CF_3$			1.36

SECTION 8

ELECTROLYTES, ELECTROMOTIVE FORCE, AND CHEMICAL EQUILIBRIUM

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EQUILIBRIUM CONSTANTS

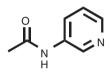
The acidities of organic compounds are typically expressed by citing their pK_A values. These are defined as $-\log_{10}K_A$ for the reaction

$$HA \rightleftharpoons H^{\oplus} + A^{\ominus}$$

The equilibrium constant K_A is defined as

$$K_A = \frac{[H^+][A^-]}{[HA]}$$

Thus, for example, the pK_A of water is $-\log_{10}([H^{\oplus}][HO^{\ominus}]/[H_2O])$ or $(10^{-7}) \cdot (10^{-7})/55.5$. The concentration of protons or hydroxide ions in water is 10^{-7} M and the concentration of water in water is 55.5 M. The equilibrium constant K_A is therefore $10^{-15.74}$. The operator "p" means " $-\log$ " so the pK_A of water is 15.7. The equilibrium constant K_W for water is 10^{-14} and is simply the product of $[H^{\oplus}] \cdot [HO^{\ominus}]$.



3-acetamidopyridine

Acidity constants are given for a range of compounds in Table 8.1. When more than one ionizable proton is present, pK_1 , pK_2 , etc. values are given. Cations formed from the indicated compound by protonation are indicated by "(+1)" or "(+2)" for a dication. For example, the dissociation of 3-acetamidopyridine is reported in Table 8.1 as "4.37(+1)." This means dissociation of the compound that is protonated (at the pyridine nitrogen atom).

Temperature values different from 25 °C are given in parentheses as are other relevant variations. For example, the dissociation constant for acetic acid- d_1 is reported in D₂O.

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C

Ionic strength μ is zero unless otherwise indicated. The protonation state of cations is designated by a value (+1), (+2), etc. that follows the pK_A value. Neutral species are indicated by (0), if it is not obvious otherwise. The charge state of anionic species is designated by (-1), (-2), etc.

Substance	pK ₁	pK ₂	pK_3	pK ₄
Abietic acid	7.62			
Acetamide	-0.37(+1)			
Acetamidine	1.60(+1)			
N-(2-Acetamido)-2-				
aminoethanesulfonic acid				
(20°C)	6.88			
2-Acetamidobenzoic acid	3.63			
3-Acetamidobenzoic acid	4.07			
4-Acetamidobenzoic acid	4.28			
2-(Acetamido)butanoic acid	3.716			
N-(2-Acetamido)iminodiacetic acid				
(20°C)	6.62			
3-Acetamidopyridine	4.37(+1)			
Acetanilide	0.4(+1)	13.39(0) ^{40°C}		
Acetic acid	4.756			
Acetic acid- d (in D_2O)	5.32			
Acetoacetic acid (18°C)	3.58			
Acetohydrazine	3.24(+1)			
Acetone oxime	12.2			
2-Acetoxybenzoic acid				
(acetylsalicylic acid)	3.48			
3-Acetoxybenzoic acid	4.00			
4-Acetoxybenzoic acid	4.38			
Acetylacetic acid (18°C)	3.58			
N-Acetyl-α-alanine	3.715			
N-Acetyl-β-alanine	4.455			
2-Acetylaminobutanoic acid	3.72			
3-Acetylaminopropionic acid	4.445			
2-Acetylbenzoic acid	4.13			
3-Acetylbenzoic acid	3.83			
4-Acetylbenzoic acid	3.70			
2-Acetylcyclohexanone	14.1			
N-Acetylcysteine (30°C)	9.52			
Acetylenedicarboxylic acid	1.75	4.40		
N-Acetylglycine	3.670			

Abietic acid

8.4 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK ₃	pK_4
N-Acetylguanidine	8.23(+1)			
N-α-Acetyl-L-histidine	7.08			
Acetylhydroxamic acid (20°C)	9.40			
N-Acetyl-2-mercaptoethylamine	9.92(SH)			
4-Acetyl-β-mercaptoisoleucine				
(30°C)	10.30			
2-Acetyl-1-naphthol (30°C)	13.40			
N-Acetylpenicillamine (30°C)	9.90			
2-Acetylphenol	9.19			
4-Acetylphenol	8.05			
2-Acetylpyridine	2.643(+1)			
3-Acetypyridine	3.256(+1)			
4-Acetylpyridine	3.505(+1)			
Aconitine	8.11(+1)			
Acridine	5.60(+1)			
Acrylic acid	4.26			
Adenine	4.17(+1)	9.75(0)		
Adeninedeoxyriboside-5'-				
phosphoric acid		4.4	6.4	
Adenine-N-oxide	2.69(+1)	8.49(0)		
Adenosine	3.5(+1)	12.34(0)		
Adenosine-5'-diphosphoric acid		4.2(-1)	7.20(-2)	
Adenosine-2'-phosphoric acid	3.81(+1)	6.17(0)		
Adenosine-3'-phosphoric acid	3.65(0)	5.88(-1)		
Adenosine-5'-phosphoric acid	3.74(0)	6.05(-1)	13.06(-2)	
Adenosine-5'-triphosphoric acid		4.00(-1)	6.48(-2)	
Adipamic acid (adipic acid				
monoamide)	4.629			
Adipic acid	4.418	5.412		
α -Alanine	2.34(+1)	9.87(0)		
β -Alanine	3.55(+1)	10.238(0)		
α -Alanine, methyl ester ($\mu = 0.10$)	7.743(+1)			
β -Alanine, methyl ester ($\mu = 0.10$)	9.170(+1)			
<i>N</i> -D-Alanyl- α -D-alanine ($\mu = 0.1$)	3.32(+1)	8.13(0)		
<i>N</i> -L-Alanyl- α -L-alanine ($\mu = 0.1$)	3.32(+1)	8.13(0)		
<i>N</i> -L-Alanyl- $lpha$ -D-alanine	3.12(+1)	8.30(0)		
N - α -Alanylglycine	3.11(+1)	8.11(0)		

N-Acetylpenicillamine

Aconitine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK ₄
Alanylglycylglycine	3.190(+1)	8.15(0)		
β -Alanylhistidine	2.64	6.86	9.40	
Albumin (bovine serum, $\mu = 0.15$)	10-10.3			
2-Aldoxime pyridine	3.42(+1)	10.22(0)		
Alizarin Black SN	5.79	12.8		
Alizarin-3-sulfonic acid	5.54	11.01		
Allantoin	8.96			
Allothreonine	2.108(+1)	9.096(0)		
Alloxanic acid	6.64			
Allylacetic acid	4.68			
Allylamine	9.69(+1)			
5-Allylbarbituric acid	4.78(+1)			
5-Allyl-5-(-methylbutyl)barbituric	8.08			
acid				
2-Allylphenol	10.28			
1-Allylpiperidine	9.65(+1)			
2-Allylpropionic acid	4.72			
3-Amidotetrazoline	3.95(+1)			
2-Aminoacetamide	7.95(+1)			
Aminoacetonitrile	5.34(+1)			
9-Aminoacridine (20°C)	9.95(+1)			
4-Aminoantipyrine	4.94(+1)			
2-Aminobenzenesulfonic acid	2.459(0)			
3-Aminobenzenesulfonic acid	3.738(0)			
4-Aminobenzenesulfonic acid	3.227(0)			
2-Aminobenzoic acid	2.09(+1)	4.79(0)		
3-Aminobenzoic acid	3.07(+1)	4.79(0)		
4-Aminobenzoic acid	2.41(+1)	4.85(0)		
2-Aminobenzoic acid, methyl ester	2.36(+1)			
3-Aminobenzoic acid, methyl ester	3.58(+1)			
4-Aminobenzoic acid, methyl ester	2.45(+1)			

4-Aminoantipyrine

9-Aminoacridine

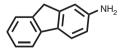
8.6 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-Aminobenzonitrile	2.75(+1)			
4-Aminobenzonitrile	1.74(+1)			
4-Aminobenzophenone	2.15(+1)			
2-Aminobenzothiazole (20°C)	4.48(+1)			
2-Aminobenzoylhydrazide	1.85	3.47	12.80	
2-Aminobiphenyl	3.78(+1)			
3-Aminobiphenyl	4.18(+1)			
4-Aminobiphenyl	4.27(+1)			
4-Amino-3-bromomethylpyridine	7.47(+1)			
4-Amino-3-bromopyridine (20°C)	7.04(+1)			
2-Aminobutanoic acid	2.286(+1)	9.830(0)		
3-Aminobutanoic acid	, ,	10.14(0)		
4-Aminobutanoic acid	4.031(+1)	10.556(0)		
2-Aminobutanoic acid, methyl ester	,			
$(\mu = 0.1)$	7.640(+1)			
4-Aminobutanoic acid, methyl ester				
$(\mu = 0.1)$	9.838(+1)			
D-(+)-2-Amino-1-butanol	9.52(+1)			
3-Amino- <i>N</i> -butyl-3-methyl-2-	7.02(11)			
butanone oxime	9.09(+1)			
4-Aminobutylphosphonic acid	2.55	7.55	10.9	
2-Amino- <i>N</i> -carbamoylbutanoic acid	3.886(+1)	7.33	10.5	
4-Amino- <i>N</i> -carbamoylbutanoic acid	4.683(+1)			
2-Amino- <i>N</i> -carbamoyl-2-				
methylpropanoic acid	4.463			
1-Amino-1-cycloheptanecarboxylic	2.59(+1)	10.46(0)		
acid	2.02(11)	100(0)		
1-Amino-1-cyclohexanecarboxylic	2.65(+1)	10.03(0)		
acid		10100(0)		
2-Amino-1-cyclohexanecarboxylic	3.56(+1)	10.21(0)		
acid				
1-Aminocyclopentane	10.65(+1)			
1-Aminocyclopropane	9.10(+1)			
10-Aminodecylphosphonic acid	7111(11)	8.0	11.25	
10-Aminodecylsulfonic acid	2.65(+1)			
1-Amino-2-di(aminomethyl)butane	3.58(+3)	8.59(+2)	9.66(+1)	
2-Amino- <i>N</i> , <i>N</i> -dihydroxyethyl-		,	,	
2-hydroxyl-1,3-propanediol	6.484(+1)			
2-Amino- <i>N</i> , <i>N</i> -dimethylbenzoic acid	1.63(+1)	8.42(0)		
4-Amino-2,5-dimethylphenol	5.28(+1)	10.40(0)		
4-Amino-3,5-dimethylpyridine (20°C)	9.54(+1)			
12-Aminododecanoic acid	4.648(+1)			
2-Aminoethane-1-phosphoric acid	5.838	10.64		
1-Aminoethanesulfonic acid	-0.33	9.06		
2-Aminoethanesulfonic acid	1.5	9.061		
2-Aminoethanethiol (cysteamine)				
$(\mu = 0.01)$	8.23(+1)			
2-Aminoethanol (ethanolamine)	9.50(+1)			
2-[2-(2-Aminoethyl)	3.50	6.59	9.51	
aminoethyl] pyridine				
				<u> </u>

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK_4
2-Amino-2-ethyl-1-butanol	9.82(+1)			
3-(2-Aminoethyl)indole		10.2		
3-Amino-N-ethyl-3-methyl-2-				
butanone oxime	9.23(+1)			
N-(2-Aminoethyl)morpholine	4.06(+2)	9.15(+1)		
p-(2-Aminoethyl)phenol	9.3	10.9		
2-Aminoethylphosphonic acid	2.45(+1)	7.0(0)	10.8(-1)	
N-(2-Aminoethyl)piperidine (30°C)	6.38	9.89		
2-(2-Aminoethyl)pyridine ($\mu = 0.5$)	4.24(+2)	9.78(+1)		
4-Amino-3-ethylpyridine (20°C)	9.51(+1)			
<i>N</i> -(2-Aminoethyl)pyrrolidine (30°C)	6.56(+2)	9.74(+1)		
2-Aminofluorine	10.34(+1)			
2-Amino-D- β -glucose ($\mu = 0.05$)	2.20(+1)	9.08(0)		
2-Amino-N-glycylbutanoic acid	3.155(+1)	8.331(0)		
7-Aminoheptanoic acid	4.502			
2-Aminohexanoic acid	2.335(+1)	9.834(0)		
6-Aminohexanoic acid	4.373(+1)	10.804(0)		
C-Amino-C-				
hydrazine	2.38(+2)	7.69(+1)		
carbonylmethane				
2-Amino-3-hydroxybenzoic acid	2.5(+1)	5.192(0)	10.118(OH)	
L-2-Amino-3-hydroxybutanoic acid				
(threonine)	2.088(+1)	9.100(0)		
DL-2-Amino-4-hydroxybutanoic acid				
$(\mu = 0.1)$	2.265(+1)	9.257(0)		
DL-4-Amino-3-hydroxybutanoic acid				
$(\mu = 0.1)$	3.834(+1)	9.487(0)		
2-Amino-2'-hydroxydiethyl sulfide	9.27(+1)			
4-Amino-2-hydroxypyrimidine				
(cytosine)	4.58(+1)	12.15(0)		
3-Amino- <i>N</i> -isopropyl-3-methyl-	, ,			
2-butanone oxime	9.09(+1)			
4-Amino-3-isopropylpyridine (20°C)	9.54(+1)			
1-Aminoisoquinoline (20°C, $\mu = 0.01$)	7.62(+1)			
3-Aminoisoquinoline				
$(20^{\circ}\text{C}, \mu = 0.005)$	5.05(+1)			
4-Aminoisoxazolidine-3-one	7.4(+1)			
Aminomalonic acid	3.32(+1)	9.83(0)		
DL-2-Amino-4-mercaptobutanoic				
acid	2.22(+1)	8.87(0)	10.86(SH)	



H_ON N OH

2-Aminofluorene

4-Amino-2-hydroxypyrimidine (cytosine)

8.8 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK_3	pK_4
2-Amino-3-mercapto-				
3-Methylbutanoic acid	1.8(+1)	7.9(0)	10.5(SH)	
2-Amino-6-methoxybenzothiazole	4.50(+1)	. , ,		
3-Amino-4-methylbenzenesulfonic				
acid	3.633			
4-Amino-3-methylbenzenesulfonic				
acid	3.125			
2-Amino-4-methylbenzothiazole	4.7(+1)			
1-Amino-3-methylbutane	10.64(+1)			
3-Amino-3-methyl-2-butanone oxime	9.09(+1)			
3-Amino-N-methyl-3-methyl-2-				
butanone oxime	9.23(+1)			
2-Amino-3-methylpentanoic acid	2.320(+1)	9.758(0)		
3-Aminomethyl-6-methylpyridine				
(30°C)	8.70(+1)			
Aminomethylphosphonic acid	2.35	5.9	10.8	
2-Amino-2-methyl-1,3-propanediol	8.801			
2-Amino-2-methyl-1-propanol	9.694(+1)			
2-Amino-2-methylpropanoic acid	2.357(+1)	10.205(0)		
(2-Aminomethyl)pyridine ($\mu = 0.5$)	2.31(+2)	8.79(+1)		
2-Amino-3-methylpyridine	7.24(+1)			
4-Amino-3-methylpyridine	9.43(+1)			
2-Amino-4-methylpyridine	7.48(+1)			
2-Amino-5-methylpyridine	7.22(+1)			
2-Amino-6-methylpyridine	7.41(+1)			
2-Amino-4-methylpyrimidine (20°C)	4.11(+1)			
Aminomethylsulfonic acid	5.75(+1)			
N-Aminomorpholine	4.19(+1)			
4-Amino-1-naphthalenesulfonic acid	2.81			
1-Amino-2-naphthalenesulfonic acid	1.71			
1-Amino-3-naphthalenesulfonic acid	3.20			
1-Amino-5-naphthalenesulfonic acid	3.69			
1-Amino-6-naphthalenesulfonic acid	3.80			
1-Amino-7-naphthalenesulfonic acid	3.66			
1-Amino-8-naphthalenesulfonic acid	5.03			
2-Amino-1-naphthalenesulfonic acid	2.35			
2-Amino-4-naphthalenesulfonic acid	3.79	0.04		
2-Amino-6-naphthalenesulfonic acid	3.79	8.94		
2-Amino-8-naphthalenesulfonic acid	3.89	4.20		
3-Amino-1-naphthoic acid	2.61	4.39		
4-Amino-2-naphthoic acid	2.89	4.46		
8-Amino-2-naphthol	4.20(+1)			
DL-2-Aminopentanoic acid	2.219(+1)	0.000		
(DL-norvaline)	2.318(+1)	9.808		
3-Aminopentanoic acid	4.02(+1)	10.399(0)		
4-Aminopentanoic acid	3.97(+1)	10.46(0)		
5-Aminopentanoic acid	4.20(+1)	9.758(0)		
5-Aminopentanoic acid, ethyl ester	10.151 9.28	9.72		
2-Aminophenol	9.20	9.12		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK ₄
3-Aminophenol	9.83	9.87		
4-Aminophenol	8.50	10.30		
4-Aminophenylacetic acid (20°C)	3.60	5.26		
2-Aminophenylarsonic acid	ca 2	3.77	8.66	
3-Aminophenylarsonic acid	ca 2	4.02	8.92	
4-Aminophenylarsonic acid	ca 2	4.02	8.62	
3-Aminophenylboric acid	4.46	8.81		
4-Aminophenylboric acid	3.71	9.17		
4-Aminophenyl				
(4-chlorophenyl) sulfone	1.38			
2-Aminophenylphosphonic acid		4.10	7.29	
3-Aminophenylphosphonic acid			7.16	
4-Aminophenylphosphonic acid			7.53	
1-Amino-1,2,3-propanetricarboxylic				
acid ($\mu = 2.2$)	2.10(+1)	3.60(0)	4.60(-1)	9.82(-2)
3-Aminopropanoic acid	3.551(+1)	10.235(0)		
1-Amino-1-propanol	9.96(+1)			
DL-2-Amino-1-propanol	9.469(+1)			
3-Amino-1-propanol	9.96(+1)			
3-Aminopropene	9.691(+1)			
3-Amino- <i>N</i> -propyl-3-methyl-				
2-butanone oxime	9.09(+1)			
2-Aminopropylsulfonic acid		9.15		
2-Aminopyridine	6.71(+1)			
3-Aminopyridine	6.03(+1)			
4-Aminopyridine	9.114(+1)			
2-Aminopyridine-1-oxide	2.58(+1)			
3-Aminopyridine-1-oxide	1.47(+1)			
4-Aminopyridine-1-oxide	3.54(+1)			
8-Aminoquinaldine	4.86(+1)			
2-Aminoquinoline (20°C, $\mu = 0.01$)	7.34(+1)			
3-Aminoquinoline (20°C, $\mu = 0.01$)	4.95(+1)			
4-Aminoquinoline (20°C, $\mu = 0.01$)	9.17(+1)			
5-Aminoquinoline (20°C, $\mu = 0.01$)	5.46(+1)			
6-Aminoquinoline (20°C, $\mu = 0.01$)	5.63(+1)			
8-Aminoquinoline (20°C, $\mu = 0.01$)	3.99(+1)			
4-Aminosalicylic acid	1.991(+1)	3.917(0)	13.74	
5-Aminosalicylic acid	2.74(+1)	5.84(0)		
2-Amino-3-sulfopropanoic acid	1.89(+1)	8.70(0)		
4-Amino-2,3,5,6-				
tetramethylpyridine (20°C)	10.58(+1)			



2-Aminopyridine-1-oxide

8-Aminoquinaldine

8.10 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK_3	pK_4
5-Amino-1,2,3,4-tetrazole (20°C)	1.76	6.07		
2-Aminothiazole (20°C)	5.36(+1)			
1-Amino-3-thiobutane (30°C)	9.18(+1)			
5-Amino-3-thio-1-pentanol (30°C)	9.12(+1)			
2-Aminothiophenol	< 2(+1)	7.90(0)		
2-Amino-4,4,4-trifluorobutanoic acid		8.171(0)		
3-Amino-4,4,4-trifluorobutanoic acid		5.831(0)		
3-Amino-2,4,6-trinitrotoluene		9.5(+1)		
Angiotensin II	10.37			
Anhydroplatynecine	9.40			
Aniline	4.60(+1)			
2-Anilinoethylsulfonic acid	3.80(+1)			
3-Anilinoethylsulfonic acid	4.85(+1)			
Anthracene-1-carboxylic acid	3.68			
Anthracene-2-carboxylic acid	4.18			
Anthracene-9-carboxylic acid	3.65			
Anthraquinone-1-carboxylic acid				
(20°C)	3.37			
Anthraquinone-2-carboxylic acid				
(20°C)	3.42			
9,10-Anthraquinone monoxime	9.78			
9,10-Anthraquinone-1-sulfonic acid	0.27			
9,10-Anthraquinone-2-sulfonic acid	0.38			
Antipyrine	1.45(+1)			
Apomorphine (15°C)		8.92		
D-(-)-Arabinose	12.34			
L-(+)-Arginine		8.994(+1)	12.47(-1)	
Arsenazo III [pK ₅ = $10.5(-4)$;			2.5	5 0(0)
$pK_6 = 12.0(-5)$		1.2	2.7	7.9(-3)
Arsenoacetic acid		4.67	7.68	
Arsenoacrylic acid		4.23	8.60	
Arsenobutanoic acid		4.92	7.64	
2-Arsenocrotonic acid		4.61	8.75	
3-Arsenocrotonic acid		4.03	8.81	
Arsenopentanoic acid	4.17	4.89	7.75	
L-(+)-Ascorbic acid (vitamin C)	4.17	11.57		
L-(+)-Asparagine		8.80(0)	0.07	
L-Asparaginylglycine		4.53	9.07	
D-Aspartic acid	7.00	3.87(0)	10.00(-)	
Aspartic diamide ($\mu = 0.2$)	7.00			



Anhydroplatynecine



Antipyrine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK_3	pK_4
Aspartylaspartic acid		3.40	4.70	8.26
α -Aspartylhistidine (38 °C, μ = 0.1)		3.02	6.82	7.98
β -Aspartylhistidine (38 °C, μ = 0.1)		2.95	6.93	8.72
<i>N</i> -Aspartyl- <i>p</i> -tyrosine ($\mu = 0.01$)		3.57	8.92	10.23(OH)
Aspidospermine	7.65			
Atropine (17°C)	4.35(+1)			
1-Azacycloheptane	11.11(+1)			
1-Azacyclooctane	11.1(+1)			
Azetidine	11.29(+1)			
Aziridine	8.04(+1)			
Barbituric acid		8.372(0)		
<i>m</i> -Benzbetaine	3.217(+1)			
p-Benzbetaine	3.245(+1)			
Benzenearsonic acid (22°C)		8.48(-1)		
Benzene-1-arsonic acid-4-carboxylic			o	
acid		4.22	5.59	
D 1 ' '1	12.7	(COOH)		
Benzeneboronic acid	13.7			
Benzene-1-carboxylic acid- 2-phosphoric acid		2.70	0.17	
2-pnospnone acid Benzene-1-carboxylic acid-		3.78	9.17	
3-phosphoric acid		4.03	7.03	
Benzene-1-carboxylic acid-		4.03	7.03	
4-phosphoric acid	1.50	3.95	6.89	
Benzenediazine	11.08(+1)	3.75	0.07	
1,3-Benzenedicarboxylic acid	11.00(+1)			
(isophthalic acid)	3.62(0)	4.60(-1)		
1,4-Benzenedicarboxylic acid	(0)	()		
(terephthalic acid)	3.54(0)	4.46(-1)		
1,3-Benzenedicarboxylic acid				
mononitrile	3.60(0)			
1,4-Benzenedicarboxylic acid	3.55(0)			
mononitrile				
Benzenehexacarboxylic acid				
$(pK_5 = 6.32; pK_6 = 7.49)$	0.68	2.21	3.52	5.09
Benzenepentacarboxylic acid				
$(pK_5 = 6.46)$	1.80	2.73	3.96	5.25
Benzenesulfinic acid	1.50			
Benzenesulfonic acid	2.554			
1,2,3,4-Benzenetetracarboxylic acid	2.05	3.25	4.73	6.21



Azetidine



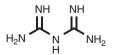
Aziridine (ethyleneimine)

8.12 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK_3	pK_4
1,2,3,5-Benzenetetracarboxylic acid	2.38	3.51	4.44	5.81
1,2,4,5-Benzenetetracarboxylic acid	1.92	2.87	4.49	5.63
1,2,3-Benzenetricarboxylic acid	2.88	4.75	7.13	
1,2,4-Benzenetricarboxylic acid	2.52	3.84	5.20	
1,3,5-Benzenetricarboxylic acid	2.12	4.10	5.18	
Benzil-α-dioxime	12.0			
Benzilic acid	3.09			
Benzimidazole	5.53(+1)	12.3(0)		
Benzohydroxamic acid (20°C)	8.89(0)			
Benzoic acid	4.204			
5,6-Benzoquinoline (20°C)	5.00(+1)			
7,8-Benzoquinoline (20°C)	4.15(+1)			
1,4-Benzoquinone monoxime	6.20			
Benzosulfonic acid	0.70			
1,2,3-Benzotriazole	8.38(+1)			
1-Benzoylacetone	8.23			
Benzoylamine	9.34(+1)			
2-Benzoylbenzoic acid	3.54			
Benzoylglutamic acid	3.49	4.99		
N-Benzoyglycine (hippuric acid)	3.65			
Benzoylhydrazine	3.03(+2)	12.45(+1)		
Benzoylpyruvic acid	6.40	12.10		
3-Benzoyl-1,1,1-trifluoroacetone	6.35			
Benzylamine	9.35(+1)			
Benzylamine-4-carboxylic acid	3.59	9.64		
2-Benzyl-2-phenylsuccinic acid				
(20°C)	3.69	6.47		
2-Benzylpyridine	5.13(+1)			
4-Benzylpyridine-1-oxide	-1.018(+)			
1-Benzylpyrrolidine	9.51(+1)			
2-Benzylpyrrolidine	10.31(+1)			
Benzylsuccinic acid (20°C)	4.11	5.65		
3-(Benzylthio)propanoic acid	4.463			
Berberine (18°C)	11.73(+1)			
Betaine	1.832(+1)			
Biguanide	2.96(+2)	11.51(+1)		
2,2'-Biimidazolyl ($\mu = 0.3$)	5.01(+1)			
2-Biphenylcarboxylic acid	3.46			





Benzilic acid

5,6-Benzoquinoline

Biguanide

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK ₃	pK_4
(1,1'-Biphenyl)-4,4'-diamine	3.63(+2)	4.70(+1)		
Bis(2-aminoethyl) ether (30°C)	8.62(+2)	9.59(+1)		
N,N'-Bis(2-aminoethyl)-		,		
ethylenediamine (20°C)	3.32(+4)	6.67(+3)	9.20(+2)	9.92(+1)
N,N-Bis(2-hydroxyethyl)-2-		\ \ \	\	
aminoethane sulfonic acid				
(BES) (20°C)	7.15			
N,N-Bis(2-hydroxyethyl)glycine				
(bicine) (20°C)	8.35			
Bis(2-hydroxyethyl)iminotris				
(hydroxymethyl)-				
methane (bis-tris)	6.46(+1)			
1,3-Bis[tris(hydroxymethyl)				
methylamino]propane (20°C)	6.80(+1)			
Bromoaetic acid	2.902			
2-Bromoaniline	2.53(+1)			
3-Bromoaniline	3.53(+1)			
4-Bromoaniline	3.88(+1)			
2-Bromobenzoic acid	2.85			
3-Bromobenzoic acid	3.810			
4-Bromobenzoic acid	3.99			
2-Bromobutanoic acid (35°C)	2.939			
erythro-2-Bromo-3-chlorosuccinic				
acid (19 °C, μ = 0.1)	1.4	2.6		
threo-2-Bromo-chlorosuccinic acid				
$(19^{\circ}C, \mu = 0.1)$	1.5	2.8		
trans-2-Bromocinnamic acid	4.41			
3-Bromo-4-(dimethylamino)pyridine				
(20°C)	6.52(+1)			
2-Bromo-4,6-dinitroaniline	-6.94(+1)			
3-Bromo-2-hydroxymethylbenzoic	` ′			
acid (20°C)	3.28			
6-Bromo-2-hydroxymethylbenzoic				
acid (20°C)	2.25			
7-Bromo-8-hydroxyquinoline-				
5-sulfonic acid	2.51	6.70		
3-Bromomandelic acid	3.13			
3-Bromo-4-methylaminopyridine				
(20°C)	7.49(+1)			
(2-Bromomethyl)butanoic acid	3.92			
Bromomethylphosphonic acid	1.14	6.52		

3-Bromomandelic acid

8.14 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2-Bromo-6-nitrobenzoic acid	1.37			
2-Bromophenol	8.452			
3-Bromophenol	9.031			
4-Bromophenol	9.34			
2-(2'-Bromophenoxy)acetic acid	3.12			
2-(3'-Bromophenoxy)acetic acid	3.09			
2-(4'-Bromophenoxy) acetic acid	3.13			
2-Bromo-2-phenylacetic acid	2.21			
2-(Bromophenyl)acetic acid	4.054			
4-(Bromophenyl)acetic acid	4.188			
4-Bromophenylarsonic acid	3.25	8.19		
4-Bromophenylphosphinic acid				
(17°C)	2.1			
2-Bromophenylphosphonic acid	1.64	7.00		
3-Bromophenylphosphonic acid	1.45	6.69		
4-Bromophenylphosphonic acid	1.60	6.83		
3-Bromophenylselenic acid	4.43			
4-Bromophenylselenic acid	4.50			
2-Bromopropanoic acid	2.971			
3-Bromopropanoic acid	3.992			
Bromopropynoic acid	1.855			
2-Bromopyridine	0.71(+1)			
3-Bromopyridine	2.85(+1)			
4-Bromopyridine	3.71(+1)			
3-Bromoquinoline	2.69(+1)			
Bromosuccinic acid	2.55	4.41		
2-Bromo- <i>p</i> -tolylphosphonic acid	1.81	7.15		
Brucine (15°C)	2.50(+2)	8.16(+1)		
2-Butanamine (<i>sec</i> -butylamine)	10.56(+1)	0.200(+1)		
1,2-Butanediamine 1.4-Butanediamine	6.399(+2) 9.35(+2)	9.388(+1) 10.82(+1)		
2.3-Butanediamine	6.91(+2)	10.82(+1) 10.00(+1)		
1,2,3,4-Butanetetracarboxylic acid	3.43	4.58	5.85	7.16
cis-2-Butenoic acid	5.45	4.36	3.63	7.10
(isocrotonic acid)	4.44			
trans-2-Butenoic acid (trans-	7.77			
crotonic acid) (35°C)	4.676			
3-Butenoic acid (vinylacetic acid)	4.68			
3-Butoxybenzoic acid (20°C)	4.25			
Butylamine	10.64(+1)			
tert-Butylamine	10.685(+1)			
4- <i>tert</i> -Butylaniline	3.78(+1)			
<i>N-tert</i> -Butylaniline	7.10(+1)			
Butylarsonic acid (18°C)	4.23	8.91		
2- <i>tert</i> -Butylbenzoic acid	3.57			
3- <i>tert</i> -Butylbenzoic acid	4.199			
4- <i>tert</i> -Butylbenzoic acid	4.389			
N-Butylethylenediamine	7.53(+2)	10.30(+1)		
<i>N</i> -Butylglycine	2.35(+1)	10.25(0)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK_4
tert-Butylhydroperoxide	12.80			
1-(<i>tert</i> -Butyl)-2-hydroxybenzene	10.62			
1-(<i>tert</i> -Butyl)-3-hydroxybenzene	10.119			
1-(<i>tert</i> -Butyl)-4-hydroxybenzene	10.23			
Butylmethylamine	10.90(+1)			
2-Butyl-1-methyl-2-pyrroline	11.84(+1)			
4- <i>tert</i> -Butylphenylactic acid	4.417			
Butylphosphinic acid	3.41			
tert-Butylphosphinic acid	4.24			
tert-Butylphosphonic acid	2.79	8.88		
1-Butylpiperidine ($\mu = 0.02$)	10.43(+1)			
2- <i>tert</i> -Butylpyridine	5.76(+1)			
3- <i>tert</i> -Butylpyridine	5.82(+1)			
4- <i>tert</i> -Butylpyridine	5.99(+1)			
2-tert-Butylthiazole ($\mu = 0.1$)	3.00(+1)			
4- <i>tert</i> -Butylthiazole ($\mu = 0.1$)	3.04(+1)			
2-Butyn-1,4-dioic acid	1.75	4.40		
2-Butynoic acid (tetrolic acid)	2.620			
Butyric acid	4.817			
4-Butyrobetaine (20°C)	3.94(+1)			
Caffeine (40°C)	10.4			
Calcein (pK ₅ $>$ 12)	<4	5.4	9.0	10.5
Calmagite	8.14	12.35		
D-Camphoric acid	4.57	5.10		
Canaline	2.40	3.70	9.20	
Canavanine	2.50(+2)	6.60(+1)	9.25(0)	
N-Carbamoylacetic acid	3.64			
N-Carbamoyl-α-D-alanine	3.89(+1)			
N-Carbamoyl-β-alanine	4.99(+1)			
DL-N-Carbamoylalanine	3.892(+1)			
N-Carbamoylglycine	3.876			
2-Carbamoylpyridine (20°C)	2.10(+1)			
3-Carbamoylpyridine	3.328(+1)			
4-Carbamoylpyridine (20°C)	3.61(+1)			
β-Carboxymethylaminopropanoic	2 (1(+1)	0.46(0)		
acid	3.61(+1)	9.46(0)		
Chloroacetic acid	2.867			
N-(2'-Chloroacetyl)glycine	3.38(0)			
cis-3-Chloroacrylic acid	2.22			
$(18^{\circ}\text{C}, \mu = 0.1)$	3.32			
trans-3-chloroacrylic acid				
$(18 ^{\circ}\text{C}, \mu = 0.1)$	3.65			
2-Chloroaniline	2.64(+1)			
3-Chloroaniline	3.52(+1)			
4-Chloroaniline	3.99(+1)			
2-Chlorobenzoic acid	2.877			
3-Chlorobenzoic acid	3.83			
4-Chlorobenzoic acid	3.986			
2-Chlorobutanoic acid	2.86			

8.16 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK ₂	pK ₃	pK ₄
		1 2	1 3	1 4
3-Chlorobutanoic acid	4.05			
4-Chlorobutanoic acid	4.50			
2-Chloro-3-butenoic acid	2.54			
3-Chlorobutylarsonic acid (18 °C)	3.95	8.85		
trans-2'-Chlorocinnamic acid	4.234			
trans-3'-Chlorocinnamic acid	4.294			
trans-4'-Chlorocinnamic acid	4.413			
2-Chlorocrotonic acid	3.14			
3-Chlorocrotonic acid	3.84			
Chlorodifluoroacetic acid	0.46			
1-Chloro-1,2-dihydroxybenzene	8.522			
1-Chloro-2,6-dimethyl-				
4-hydroxybenzene	9.549			
4-Chloro-2,6-dinitrophenol	2.97			
2-Chloroethylarsonic acid	3.68	8.37		
3-Chlorohexyl-1-arsonic acid (18°C)	3.51	8.31		
2-Chloro-3-hydroxybutanoic acid	2.59			
3-Chloro-2-(hydroxymethyl)benzoic				
acid (20°C)	3.27			
6-Chloro-2-(hydroxymethyl)benzoic				
acid (20°C)	2.26			
7-Chloro-8-hydroxyquinoline-				
5-sulfonic acid	2.92	6.80		
2-Chloroisocrotonic acid	2.80			
3-Chloroisocrotonic acid	4.02			
3-Chlorolactic acid	3.12			
3-Chloromandelic acid	3.237			
3-Chloro-4-methoxyphenyl-				
phosphonic acid	2.25	6.7		
3-Chloro-4-methylaniline	4.05(+1)	0.7		
4-Chloro- <i>N</i> -methylaniline	3.9(+1)			
4-Chloro-3-methylphenol	9.549			
Chloromethylphosphonic acid	1.40	6.30		
2-Chloro-2-methylpropanoic acid	2.975	0.50		
2-Chloro-6-nitroaniline	-2.41(+1)			
4-Chloro-2-nitroaniline	-1.10(+1)			
2-Chloro-3-nitrobenzoic acid	2.02			
2-Chloro-4-nitrobenzoic acid	1.96			
2-Chloro-5-nitrobenzoic acid	2.17			
2-Chloro-6-nitrobenzoic acid	1.342			
4-Chloro-2-nitrophenol	6.48			
4-Cinoro-2-introphenor	0.40	I	I	I

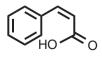
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK ₄
2-Chlorophenol	8.55			
3-Chlorophenol	9.10			
4-Chlorophenol	9.43			
(4-Chloro-3-nitrophenoxy)acetic acid	2.959			
2-Chloro-4-nitrophenylphosphonic				
acid	1.12	6.14		
3-Chloropentyl-l-arsonic acid				
(18°C)	3.71	8.77		
2-Chlorophenoxyacetic acid	3.05			
3-Chlorophenoxyacetic acid	3.07			
4-Chlorophenoxyacetic acid	3.10			
4-Chlorophenoxy-2-methylacetic				
acid	3.26			
2-Chlorophenylacetic acid	4.066			
3-Chlorophenylacetic acid	4.140			
4-Chlorophenylacetic acid	4.190			
2-Chlorophenylalanine	2.23(+1)	8.94(0)		
3-Chlorophenylalanine	2.17(+1)	8.91(0)		
DL-4-Chlorophenylalanine	2.08(+1)	8.96(0)		
4-Chlorophenylarsonic acid	3.33	8.25		
2-Chlorophenylphosphonic acid	1.63	6.98		
3-Chlorophenylphosphonic acid	1.55	6.65		
4-Chlorophenylphosphonic acid	1.66	6.75		
3-(2'-Chlorophenyl)propanoic acid	4.577			
3-(3'-Chlorophenyl)propanoic acid	4.585			
3-(4'-Chlorophenyl)propanoic acid	4.607			
3-Chlorophenylselenic acid	4.47			
4-Chlorophenylselenic acid	4.48			
4-Chloro-1,2-phthalic acid	1.60			
2-Chloropropanoic acid	2.84			
3-Chloropropanoic acid	3.992			
2-Chloropropylarsonic acid (18°C)	3.76	8.39		
3-Chloropropylarsonic acid (18°C)	3.63	8.53		
Chloropropynoic acid	1.845			
2-Chloropyridine	0.49(+1)			
3-Chloropyridine	2.84(+1)			
4-Chloropyridine	3.83(+1)			
7-Chlorotetracycline	3.30(+1)	7.44	9.27	
4-Chloro-2-(2'-thiazolylazo)phenol	7.09			
4-Chlorothiophenol	5.9			
N-Chloro- <i>p</i> -toluenesulfonamide	4.54(+1)			
3-Chloro-o-toluidine	2.49(+1)			
4-Chloro-o-toluidine	3.385(+1)			
5-Chloro-o-toluidine	3.85(+1)			
6-Chloro-o-toludine	3.62(+1)			
Chrome Azurol S	2.45	4.86	11.47	
Chrome Dark Blue	7.56	9.3	12.4	
Cinchonine	5.85(+2)	9.92(+1)		

8.18 SECTION 8

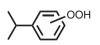
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK_3	pK ₄
cis-Cinnamic acid	3.879			
trans-Cinnamic acid	4.438			
Citraconic acid	2.29(0)	6.15(-1)		
Citric acid	3.128	4.761	6.396	
L-(+)-Citrulline	2.43(+1)	9.41(0)		
Cocaine	8.41(+1)			
Codeine	7.95(+1)			
Colchicine	1.65(+1)			
Coniine ($\mu = 0.5$)	11.24(+1)			
Creatine (40°C)	3.28(+1)			
Creatinine	3.57(+1)			
o-Cresol	10.26			
m-Cresol	10.00			
p-Cresol	10.26			
Cumene hydroperoxide	12.60			
Cupreine	7.63(+1)			
Cyanamide	10.27			
Cyanoacetic acid	2.460			
Cyanoacetohydrazide	2.34(+2)	11.17(+1)		
2-Cyanobenzoic acid	3.14			
3-Cyanobenzoic acid	3.60			
4-Cyanobenzoic acid	3.55			
4-Cyanobutanoic acid	4.44			
trans-1-Cyanocyclohexane-				
2-carboxylic acid	3.865			
4-Cyano-2,6-dimethylphenol	8.27			
4-Cyano-3,5-dimethylphenol	8.21			
2-Cyanoethylamine	7.7(+1)			
N-(2-Cyano)ethylnorcodeine	5.68(+1)			
Cyanomethylamine	5.34(+1)			
2-Cyano-2-methyl-2-phenylacetic				
acid	2.290			
1-Cyanomethylpiperidine	4.55(+1)			
2-Cyano-2-methylpropanoic acid	2.422			
3-Cyanophenol	8.61			
o-Cyanophenoxyacetic acid	2.98			
m-Cyanophenoxyacetic acid	3.03			
p-Cyanophenoxyacetic acid	2.93			
2-Cyanopropanoic acid	2.37			
3-Cyanopropanoic acid	3.99			
2-Cyanopyridine	-0.26(+1)			



OHOOHO





cis-Cinnamic acid

Citraconic acid

Citric acid

Cumene hydroperoxide

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK ₄
3-Cyanopyridine	1.45(+1)			
4-Cyanopyridine	1.90(+1)			
Cyanuric acid	6.78			
Cyclobutanecarboxylic acid	4.785			
1,1-Cyclobutanedicarboxylic acid	3.13	5.88		
cis-1,2-Cyclobutanedicarboxylic acid	3.90	5.89		
trans-1,2-Cyclobutanedicarboxylic				
acid	3.79	5.61		
cis-1,3-Cyclobutanedicarboxylic acid	4.04	5.31		
trans-1,3-Cyclobutanedicarboxylic				
acid	3.81	5.28		
Cyclohexanecarboxylic acid	4.90			
1,1-Cyclohexanediacetic acid	3.49	6.96		
cis-1,2-Cyclohexanediacetic acid				
(20°C)	4.42	5.45		
trans-1,2-Cyclohexanediacetic acid				
(20°C)	4.38	5.42		
cis-1,2-Cyclohexanediamine	6.43(+2)	9.93(+1)		
trans-1,2-Cyclohexanediamine	6.34(+2)	9.74(+1)		
1,1-Cyclohexanedicarboxylic acid	3.45	4.11		
cis-1,2-Cyclohexanedicarboxylic acid				
(20°C)	4.34	6.76		
trans-1,2-Cyclohexanedicarboxylic				
acid (20°C)	4.18	5.93		
cis-1,3-Cyclohexanedicarboxylic acid				
(16°C)	4.10	5.46		
trans-1,3-Cyclohexanedicarboxylic				
acid (19°C)	4.31	5.73		
trans-1,4-Cyclohexanedicarboxylic				
acid (16°C)	4.18	5.42		
1,3-Cyclohexanedione	5.26	02		
cis, cis-1,3,5-Cyclohexanetriamine	6.9(+3)	8.7(+2)	10.4(+1)	
Cyclohexanonimine	9.15	0.7(12)	10(+1)	
cis-4-Cyclohexene-1,2-dicarboxylic				
acid (20°C)	3.89	6.79		
trans-4-Cyclohexene-1,2-dicarboxylic	0.05	""		
acid (20°C)	3.95	5.81		
Cyclohexylacetic acid	4.51	3.01		
Cyclohexylamine	10.64(+1)			
2-(Cyclohexylamino)ethanesulfonic	-0.0.(. 1)			
acid (CHES) (20°C)	9.55			

$$HO \stackrel{N}{\longleftarrow} N \stackrel{OH}{\longleftarrow} N$$

Cyanuric acid

8.20 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK_4
3-Cyclohexylamino-				
1-propanesulfonic acid (CAPS)				
(20°C)	10.40			
4-Cyclohexylbutanoic acid	4.95			
Cyclohexylcyanoacetic acid	2.367			
1,2-Cyclohexylenedinitriloacetic acid				
$(\mu = 0.1)$	2.4	3.5	6.16	12.35
3-Cyclohexylpropanoic acid	4.91			
2-Cyclohexylpyrrolidine	10.76(+1)			
2-Cyclohexyl-2-pyrroline	7.91(+1)			
Cyclohexylthioacetic acid	3.488			
Cyclopentanecarboxylic acid	4.905			
cis-Cyclopentane-1-carboxylic acid-				
2-acetic acid	4.40	5.79		
trans-Cyclopentane-1-carboxylic				
acid-2-acetic acid	4.39	5.67		
Cyclopentane-1,2-diamine-N,N',N'-				
tetraacetic acid ($\mu = 0.1$)				10.20
Cyclopentane-1,1-dicarboxylic acid	3.23	4.08		
cis-Cyclopentane-1,2-dicarboxylic				
acid	4.43	6.67		
trans-Cyclopentane-1,2-dicarboxylic				
acid	3.96	5.85		
cis-Cyclopentane-1,3-dicarboxylic				
acid	4.26	5.51		
trans-Cyclopentane-1,3-dicarboxylic				
acid	4.32	5.42		
Cyclopentylamine	10.65(+1)			
1,1-Cyclopentyldiacetic acid	3.80	6.77		
cis-Cyclopentyl-1,2-diacetic acid	4.42	5.42		
trans-Cyclopentyl-1,2-diacetic acid	4.43	5.43		
Cyclopropanecarboxylic acid	4.827			
Cyclopropane-1,1-dicarboxylic acid	1.82	5.43		
cis-Cyclopropane-1,2-dicarboxylic				
acid	3.33	6.47		
trans-Cyclopropane-1,2-dicarboxylic				
acid	3.65	5.13		
Cyclopropylamine	9.10(+1)			
5-Cyclopropyl-1,2,3,4-tetrazole	4.90(+1)			
L-Cysteic acid (3-sulfo-L-alanine)	1.89(+1)	8.7(0)		
L-(+)-Cysteine	1.71(+1)	8.39(0)	10.70(SH)	



5-Cyclopropyl-1,2,3,4-tetrazole

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
L-(+)-Cysteine, ethyl ester	6.69	9.17(SH)		
	(NH ₃ ⁺)			
L-(+)-Cysteine, methyl ester	6.56	8.99(SH)		
L-Cysteinyl-L-asparagine	(NH ₃ ⁺) 2.97	7.09	8.47	
L-Cystine (35°C)	1.6(+2)	2.1(+1)	8.02(0)	8.71(-1)
Cystinylglycylglycine (35 °C)	3.12	3.21	6.01	6.87
Cytidine	4.08(+1)	12.24(0)		
Cytidine-2'-phosphoric acid	0.8(+1)	4.36(0)	6.17(-1)	
Cytidine-3'-phosphoric acid	0.80(+1)	4.31(0)	6.04(-1)	13.2(sugar)
Cytidine-5'-phosphoric acid		4.39(0)	6.62(-1)	
Cytosine	4.58(+1)	12.15(0)		
Decanedioic acid (sebacic acid)	4.59	5.59		
Dehydroascorbic acid (20°C)	3.21	7.92	10.3	
2'-Deoxyadenosine ($\mu = 0.1$)	3.8(+1)			
Deoxycholic acid	6.58			
2-Deoxyglucose	12.52			
2-Deoxyguanosine ($\mu = 0.1$)	2.5(+1)			
5-Desoxypyridoxal ($\mu = 0$)	4.17(+1)	8.14(OH)		
1,1-Diacetic acid semicarbazide				
$(30^{\circ}\text{C}, \mu = 0.1)$	2.96	4.04		
Diacetylacetone	7.42			
Diallylamine ($\mu = 0.02$)	9.29(+1)			
5,5-Diallylbarbituric acid	7.78(0)	0.56(+0)	10.20(+1)	
1,3-Diamino-2-aminomethylpropane	6.44(+3)	8.56(+2)	10.38(+1)	
3,5-Diaminobenzoic acid 1,3-Diamino- <i>N</i> , <i>N</i> ′-bis-	5.30			
(2-aminoethyl)propane ($\mu = 0.5$)	6.01(+4)	7.26(+3)	9.49(+2)	10.23(+1)
2,4-Diaminobutanoic acid (20°C)	1.85(+2)	8.24(+1)	10.40(0)	10.23(+1)
2,2'-Diaminodiethyl sulfide (30°C)	8.84(+2)	9.64(+1)	10.10(0)	
1,8-Diamino-3,6-dithiooctane (30°C)	8.43(+2)	9.31(+1)		
2,7-Diaminooctanedioic acid	0110(12)	7.000(1.0)		
$(20^{\circ}\text{C}, \mu = 0.1)$	1.84(+2)	2.64(+1)	9.23(0)	9.89(-1)
1,8-Diamino-3,6-octanedione (30°C)	8.60(+2)	9.57(+1)	` /	\ \ \ \ \ \
1,8-Diamino-3-oxa-6-thiooctane	8.54(+2)	9.46(+1)		
2,3-Diaminopropanoic acid ($\mu = 0.1$)	1.33(+2)	6.674(+1)	9.623(0)	
2,3-Diaminopropanoic acid, methyl				
ester ($\mu = 0.1$)	4.412(+1)	8.250(0)		
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			OH	

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Deoxycholic acid

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK ₃	pK_4
1,3-Diamino-2-propanol (20°C)	7.93(+2)	9.69(+1)		
2,5-Diaminopyridine (20°C)	2.13(+2)	6.48(+1)		
1,4-Diazabicyclo[2.2.2]octane	2.90(+2)	8.60(+1)		
Dibenzylamine	8.52(+1)	. ,		
Dibenzylsuccinic acid (20°C)	3.96	6.66		
Dibromoacetic acid	1.39			
3,5-Dibromoaniline	2.35(+1)			
3,5-Dibromophenol	8.056			
2,2-Dibromopropanoic acid	1.48			
2,3-Dibromopropanoic acid	2.33			
rac-2,3-Dibromosuccinic acid				
(20°C)	1.43	2.24		
meso-2,3-Dibromosuccinic acid				
(20°C)	1.51	2.71		
3,5-Dibromo- <i>p</i> -L-tyrosine	2.17(+1)	6.45(0)	7.60(-1)	
Dibutylamine	11.25(+1)		, ,	
Di-sec-butylamine	10.91(+1)			
2,6-Di- <i>tert</i> -butylpyridine	3.58(+1)			
rac-2,3-Di-tert-butylsuccinic acid	. ,			
$(\mu = 0.1)$	3.58	10.2		
1,12-Dicarboxydodecaborane	9.07	10.23		
Dichloroacetic acid	1.26			
Dichloroacetylacetic acid	2.11			
3,5-Dichloroaniline	2.37(+1)			
1,3-Dichloro-2,5-dihydroxybenzene	. ,			
$(\mu = 0.65)$	7.30	9.99		
2,5-Dichloro-3,6-dihydroxy-				
<i>p</i> -benzoquinone	1.09	2.42		
Dichloromethylphosphonic acid	1.14	5.61		
2,4-Dichloro-6-nitroaniline	-3.00(+1)			
2,5-Dichloro-4-nitroaniline	-1.74(+1)			
2,6-Dichloro-4-nitroaniline	-3.31(+1)			
2,3-Dichlorophenol	7.44			
2,4-Dichlorophenol	7.85			
2,6-Dichlorophenol	6.78			
3,4-Dichlorophenol	8.630			
3,5-Dichlorophenol	8.179			
2,4-Dichlorophenoxyacetic acid				
(2,4-D)	2.64			
4,6-Dichlorophenoxy-2-methylacetic				
acid	3.13			
3,6-Dichlorophthalic acid	1.46			
2,2-Dichloropropanoic acid	2.06			
2,3-Dichloropropanoic acid	2.85			
rac-2,3-Dichlorosuccinic acid (20°C)	1.43	2.81		
meso-2,3-Dichlorosuccinic acid	1.49	2.97		
3,5-Dichloro- <i>p</i> -tyrosine	2.12	6.47	7.62	
2-Dicyanoethylamine	5.14(+1)			
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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK_3	pK_4
Dicyclohexylamine	11.25(+1)			
Dicyclopentylamine	10.93(+1)			
Didodecylamine	10.99(+)			
Diethanolamine	8.88(+1)			
Di(ethoxyethyl)amine	8.47(+1)			
3,5-Diethoxyphenol	9.370			
3-(Diethoxyphosphinyl)benzoic acid	3.65			
4-(Diethoxyphosphinyl)benzoic acid	3.60			
3-(Diethoxyphosphinyl)phenol	8.66			
4-(Diethoxyphosphinyl)phenol	8.28			
Diethylamine	10.8(+1)			
2-(Diethylamino)ethyl-	l ` ´			
4-aminobenzoate	8.85(+1)			
α -(Diethylamino)toluene	9.44(+1)			
<i>N</i> , <i>N</i> -Diethylaniline	6.56(+1)			
5,5-Diethylbarbituric acid (veronal)	8.020(0)			
<i>N,N</i> -Diethylbenzylamine	9.48(+1)			
Diethylbiguanide (30°C)	2.53(+1)	11.68(0)		
Diethylenetriamine	4.42(+3)	9.21(+2)	10.02(+1)	
Diethylenetriaminepentaacetic acid	l ` ´		` ´ ĺ	
$(pK_5 = 10.58)$	1.80(0)	2.55(-1)	4.33(-2)	8.60(-3)
<i>N,N</i> -Diethylethylenediamine	7.70(+2)	10.46(+1)	, ,	, ,
2,2-Diethylglutaric acid	3.62	7.12		
<i>N,N</i> -Diethylglycine	2.04(+1)	10.47(0)		
Diethylglycolic acid (18°C)	3.804			
Diethylmalonic acid	2.151	7.417		
Diethylmethylamine	10.43(+1)			
rac-2,3-Diethylsuccinic acid	3.63	6.46		
meso-2,3-Diethylsuccinic acid	3.54	6.59		
<i>N</i> , <i>N</i> -Diethyl- <i>o</i> -toluidine	7.18(+1)			
Difluoroacetic acid	1.33			
3,3-Difluoroacrylic acid	3.17			
Diglycolic acid	2.96			
Diguanidine	12.8			
Dihexylamine	11.0(+1)			
Dihydroarecaidine	9.70			
Dihydroarecaidine, methyl ester	8.39			
Dihydrocodeine	8.75(+1)			
Dihydroergonovine	7.38(+1)			
α -Dihydrolysergic acid	3.57	8.45		

Dihydroarecaidine

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
γ-Dihydrolysergic acid	3.60	8.71		
α-Dihydrolysergol	8.30			
β-Dihydrolysergol	8.23			
Dihydromorphine	9.35			
3,4-Dihydroxyalanine	2.32(+1)	8.68(0)	9.87(-1)	
1,2-Dihydroxyanthraquinone-			,	
3-sulfonic acid				
(alizarin-3-sulfonic acid)		5.54(-1)	11.01(-2)	
3,4-Dihydroxybenzaldehyde	7.55	\ \ \ \	` /	
1,2-Dihydroxybenzene				
(pyrocatechol) ($\mu = 0.1$)	9.356(0)	12.98(-1)		
1,3-Dihydroxybenzene (resorcinol)	9.44(0)	12.32(-1)		
1,4-Dihydroxybenzene		\ \ \ \ \ \ \ \ \		
(hydroquinone)	9.91(0)	12.04(-1)		
4,5-Dihydroxybenzene-1,3-disulfonic	. ,	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \		
acid			7.66(-2)	12.6(-3)
2,3-Dihydroxybenzoic acid (30°C)	2.98	10.14	` ′	
2,4-Dihydroxybenzoic acid				
(β-resorcyclic acid)	3.29	8.98		
2,5-Dihydroxybenzoic acid	2.97	10.50		
2,6-Dihydroxybenzoic acid	1.30			
3,4-Dihydroxybenzoic acid	4.48	8.67	11.74	
3,5-Dihydroxybenzoic acid	4.04			
2,5-Dihydroxy- <i>p</i> -benzoquinone	2.71	5.18		
3,4-Dihydroxy-3-cyclobutene-				
1,2-dione	0.541	3.480		
2,3-Dihydroxy-2-cyclopenten-1-one				
(20°C)	4.72			
1,4-Dihydroxy-2,6-dinitrobenzene	4.42	9.14		
Di(2,2'-hydroxyethyl)amine	8.8(+1)			
N,N-Di(2-hydroxyethyl)glycine	8.333			
Dihydroxymaleic acid	1.10			
Dihydroxymalic acid	1.92			
1,3-Dihydroxy-2-methylbenzene				
$(\mu = 0.65)$	10.05	11.64		
2,2-Di(hydroxymethyl)-				
3-hydroxypropanoic acid	4.460			
2,4-Dihydroxy-5-methylpyrimidine	9.90			
2,4-Dihydroxy-6-methylpyrimidine	9.52			
1,4-Dihydroxynaphthalene				
$(26^{\circ}\text{C}, \mu = 0.65)$	9.37	10.93		
1,2-Dihydroxy-3-nitrobenzene	6.68			
1,2-Dihydroxy-4-nitrobenzene				
$(\mu = 0.1)$	6.701			
2,4-Dihydroxy-1-phenylazobenzene				
$(\mu = 0.1)$	11.98			
2,4-Dihydroxyoxazolidine	6.11(+1)			
2,4-Dihydroxypteridine	< 1.3	7.92		
2,6-Dihydroxypurine	7.53(0)	11.84(-1)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK_4
2,4-Dihydroxypyridine (20°C)	1.37(+1)	6.45(0)	13(-1)	
Dihydroxytartaric acid	1.95	4.00	` ′	
1,4-Dihydroxy-2,3,5,6-				
tetramethylbenzene ($\mu = 0.65$)	11.25	12.70		
3,5-Diiodoaniline	2.37(+1)			
2,5-Diiodohistamine	2.31(+2)	8.20(+1)	10.11(0)	
2,5-Diiodohistidine ($\mu = 0.1$)	2.72	8.18	9.76	
3,5-Diiodophenol	8.103			
3,5-Diiodotyrosine	2.117(+1)	6.479(0)	7.821(-1)	
Diisopropylmalonic acid	2.124	8.848		
Dilactic acid	2.955			
threo-1,4-Dimercapto-2,3-butanediol	8.9			
meso-2,3-Dimercaptosuccinic acid	2.71	3.48	8.89(SH)	10.79(SH)
3,5-Dimethoxyaniline	3.86(+1)			
2,6-Dimethoxybenzoic acid	3.44			
1,10-Dimethoxy-3,8-dimethyl-				
4,7-phenanthroline	7.21			
Di(2-methoxyethyl)amine	9.51(+1)			
3,5-Dimethoxyphenol	9.345			
(3,4-Dimethoxy)phenylacetic acid	4.333			
Dimethylamine	10.77(+1)			
4-Dimethylaminobenzaldehyde	1.647(+1)			
N,N-Dimethylaminocyclohexane	10.72(+1)			
4-Dimethylamino-2,3-dimethyl-				
1-phenyl-3-pyrazolin-5-one	4.18(+1)			
4-Dimethylamino-				
3,5-dimethylpyridine (20°C)	8.15(+1)			
2-(Dimethylamino)ethanol	9.26(+1)			
2-[2-(Dimethylamino)ethyl]pyridine	3.46(+2)	8.75(+1)		
3-(Dimethylaminoethyl)pyridine	4.30(+2)	8.86(+1)		
4-(Dimethylaminoethyl)pyridine	4.66(+2)	8.70(+1)		
4-(Dimethylamino)-3-ethylpyridine				
(20°C)	8.66(+1)			
4-(Dimethylamino)-				
3-isopropylpyridine (20°C)	8.27(+1)			
2-(Dimethylaminomethyl)pyridine	2.58(+2)	8.12(+1)		
3-(Dimethylaminomethyl)pyridine	3.17(+2)	8.00(+1)		
4-(Dimethylaminomethyl)pyridine	3.39(+2)	7.66(+1)		
4-(Dimethylamino)-3-methylpyridine				
(20°C)	8.68(+1)			
4-(Dimethylaminophenyl)phosphonic				
acid	2.0(+1)	4.2	7.35	
3-(Dimethylamino)propanoic acid	9.85(+1)			
4-(Dimethylamino)pyridine (20°C)	6.09(+1)			
<i>N,N</i> -Dimethylaniline	5.15(+1)			
2,3-Dimethylaniline	4.70(+1)			
2,4-Dimethylaniline	4.89(+1)			
2,5-Dimethylaniline	4.53(+1)			
2,6-Dimethylaniline	3.95(+1)			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK_4
3,4-Dimethylaniline	5.17(+1)			
3,5-Dimethylaniline	4.765(+1)			
N,N-Dimethylaniline-4-phosphonic				
acid (17°C)	2.0(+1)	4.2	7.39	
Dimethylarsinic acid (cacodylic acid)	6.273			
1,3-Dimethylbarbituric acid	4.68(+1)			
2,3-Dimethylbenzoic acid	3.771			
2,4-Dimethylbenzoic acid	4.217			
2,5-Dimethylbenzoic acid	3.990			
2,6-Dimethylbenzoic acid	3.362			
3,4-Dimethylbenzoic	4.41			
3,5-Dimethylbenzoic acid	4.302			
N,N-Dimethylbenzylamine	9.02(+1)	11.50		
Dimethylbiguanide	2.77(+1)	11.52		
2,2-Dimethylbutanoic acid (18°C)	5.03			
Dimethylchlorotetracycline ($\mu = 0.01$) 2,6-Dimethyl-4-cyanophenol	3.30(+1)			
	8.27			
3,5-Dimethyl-4-cyanophenol	8.21 5.15			
5,5-Dimethyl-1,3-cyclohexanedione <i>cis</i> -3,3-Dimethyl-1,2-	3.13			
cyclopropanedicarboxylic acid	2.34	8.31		
trans-3,3-Dimethyl-	2.34	0.31		
1,2-cyclopropanedicarboxylic acid	3.92	5.32		
3,5-Dimethyl-4-(dimethylamino)-	3.92	3.32		
pyridine (20°C)	8.12(+1)			
2,2-Dimethyl-1,3-dioxane-4,6-dione	5.1			
1,1-Dimethylethanethiol ($\mu = 0.1$)	11.22			
N,N-Dimethylethylenediamine-	11.22			
N,N-diacetic acid	6.63	9.53		
<i>N</i> , <i>N'</i> -Dimethylethylenediamine-	0.03	7.55		
N,N'-diacetic acid	7.40	10.16		
N,N-Dimethylethylenediamine-	7.40	10.10		
N,N'-diacetic acid	5.99	9.97		
N,N-Dimethylglycine	2.146(+1)	9.940(0)		
Dimethylglycolic acid (18°C)	4.04).5 10(0)		
N,N-Dimethylglycylglycine	3.11(+1)	8.09(0)		
Dimethylglyoxime	10.60	0.05(0)		
5,5-Dimethyl-2,4-hexanedione	10.01			
5,5-Dimethylhydantoin	9.19			
2,4-Dimethyl-8-hydroxyquinoline	6.20(+1)	10.60(0)		
3,4-Dimethyl-8-hydroxyquinoline	5.80(+1)	10.05(0)		

Dimethylglyoxime

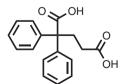
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK ₂	\mathbf{pK}_3	pK_4
2,4-Dimethyl-8-hydroxyquinoline-				
7-sulfonic acid	3.20	10.14(OH)		
	(NH ⁺)			
Dimethylhydroxytetracycline	7.5	9.4		
2,4-Dimethylimidazole	8.38(+1)			
Dimethylmalic acid	3.17	6.06		
2,2-Dimethylmalonic acid	3.17	6.06		
3,5-Dimethyl-4-(methylamino)				
pyridine (20°C)	9.96(+1)			
2,3-Dimethylnaphthalene-				
1-carboxylic acid	3.33			
2,6-Dimethyl-4-nitrophenol	7.190			
3,5-Dimethyl-4-nitrophenol	8.245			
α, α -Dimethyloxaloacetic acid	1.77	4.62		
3,3-Dimethylpentanedioic acid	3.70	6.34		
2,2-Dimethylpentanoic acid	4.969			
4,4-Dimethylpentanoic acid (18°C)	4.79			
2,3-Dimethylphenol	10.50			
2,4-Dimethylphenol	10.58			
2,5-Dimethylphenol	10.22			
2,6-Dimethylphenol	10.59			
3,4-Dimethylphenol	10.32			
3,5-Dimethylphenol	10.15			
2,6-Dimethylphenoxyacetic acid	3.356			
Dimethylphenylsilylacetic acid	5.27			
<i>N</i> , <i>N</i> ′-Dimethylpiperazine	4.630(+2)	8.539(+1)		
1,2-Dimethylpiperidine	10.22			
cis-2,6-Dimethylpiperidine	11.07(+1)			
2,2-Dimethylpropanoic acid				
(pivalic acid)	5.031			
2,2'-Dimethylpropylphosphonic acid	2.84	8.65		
2,4-Dimethylpyridine (2,4-lutidine)	6.74(+1)			
2,5-Dimethylpyridine (2,5-lutidine)	6.43(+1)			
2,6-Dimethylpyridine (2,6-lutidine)	6.71(+1)			
3,4-Dimethylpyridine (3,4-lutidine)	6.47(+1)			
3,5-Dimethylpyridine (3,5-lutidine)	6.09(+1)			
2,4-Dimethylpyridine-1-oxide	1.627(+1)			
2,5-Dimethylpyridine-1-oxide	1.208(+1)			
2,6-Dimethylpyridine-1-oxide	1.366(+1)			
3,4-Dimethylpyridine-1-oxide	1.493(+1)			
3,5-Dimethylpyridine-1-oxide	1.181(+1)			
2,3-Dimethylquinoline	4.94(+1)			
2,6-Dimethylquinoline	5.46(+1)			
meso-2,2-Dimethylsuccinic acid	3.77	5.936		
rac-2,2-Dimethylsuccinic acid	3.93	6.20		
D-2,3-Dimethylsuccinic acid	3.82	5.93		
meso-2,3-Dimethylsuccinic acid	3.67	5.30		
rac-2,3-Dimethylsuccinic acid	3.94	6.20		
2,4-Dimethylthiazole ($\mu = 0.1$)	3.98			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK ₃	pK_4
2,5-Dimethylthiazole ($\mu = 0.1$)	3.91			
4,5-Dimethylthiazole ($\mu = 0.1$)	3.73			
N,N-Dimethyl-o-toluidine	5.86(+1)			
<i>N,N</i> -Dimethyl- <i>p</i> -toluidine	7.24(+1)			
2,4-Dinitroaniline	-4.25(+1)			
2,6-Dinitroaniline	-5.23(+1)			
3,5-Dinitroaniline	0.229(+1)			
2,3-Dinitrobenzoic acid	1.85			
2,4-Dinitrobenzoic acid	1.43			
2,5-Dinitrobenzoic acid	1.62			
2,6-Dinitrobenzoic acid	1.14			
3,4-Dinitrobenzoic acid	2.82			
3,5-Dinitrobenzoic acid	2.85			
1,1-Dinitrobutane (20°C)	5.90			
1,1-Dinitrodecane	3.60			
1,1-Dinitroethane (20°C)	5.21			
Dinitromethane (20°C)	3.60			
1,1-Dinitropentane	5.337			
2,4-Dinitrophenol	4.08			
2,5-Dinitrophenol	5.216			
2,6-Dinitrophenol	3.713			
3,4-Dinitrophenol	5.424			
3,5-Dinitrophenol	6.732			
2,4-Dinitrophenylacetic acid	3.50			
1,1-Dinitropropane (20°C)	5.5			
2,6-Dioxo-1,2,3,6-tetrahydro-				
4-pyrimidinecarboxylic acid				
(orotic acid)	1.8(+1)	9.55(0)		
Diphenylacetic acid	3.939			
Diphenylamine	0.9(+1)			
2,2-Diphenylglutaric acid (20°C)	3.91	5.38		
1,3-Diphenylguanidine	10.12			
2,2-Diphenylheptanedioic acid				
(20°C)	4.28	5.39		
2,2-Diphenylhexanedioic acid (20°C)	4.17	5.40		
3,3-Diphenylhexanedioic acid	4.22	5.19		
Diphenylhydroxyacetic acid (35°C)	3.05			
Diphenylketimine	6.82			
2,2-Diphenylnonanedioic acid (20°C)	4.33	5.38		





2,2-Diphenylglutaric acid

Diphenylketimine

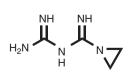
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK ₂	pK_3	pK_4
meso-2,2-Diphenylsuccinic acid	3.48			
rac-2,2-Diphenylsuccinic acid	3.58			
2,2-Diphenylsuccinic acid, 1-methyl				
ester (20°C)	4.47			
2,2-Diphenylsuccinic acid, 4-methyl				
ester (20°C)	3.900			
Diphenylthiocarbazone	4.50	15		
Dipropylamine	10.91(+1)			
Dipropylenetriamine	7.72(+3)	9.56(+2)	10.65(+1)	
2,2-Dipropylglutaric acid	3.688	7.31		
Dipropylmalonic acid	2.04	7.51		
2,2'-Dipyridyl	-0.52(+2)	4.352(+1)		
2,3'-Dipyridyl (20°C)	1.52(+2)	4.42(+1)		
2,4'-Dipyridyl (20°C)	1.19(+2)	4.77(+1)		
$3.3'$ -Dipyridyl (20°C, $\mu = 0.2$)	3.0(+2)	4.60(+1)		
3,4'-Dipyridyl (20°C, $\mu = 0.2$)	3.0(+2)	4.85(+1)		
4,4'-Dipyridyl	3.17(+2)	4.82(+1)		
Dithiodiacetic acid (18°C)	3.075	4.201		
1,4-Dithioerythritol	9.5			
Dithiooxamide (rubeanic acid)	10.89			
Dulcitol	13.46			
Ecgonine	10.91			
Emetine	7.36(+1)	8.23(0)		
Epinephrine enantiomorph	9.39(+1)			
Epinephrine, pseudo	9.53(+1)			
Ergometrinine	7.32(+1)			
Ergonovine	6.73(+1)			
Eriochrome Black T	6.3	11.55		
1,2-Ethanediamine	6.85(+2)	9.92(+1)		
Ethane-1,2-diamino-N,N'-dimethyl-				
<i>N</i> , <i>N</i> ′-diacetic acid (20 °C)	6.047(0)	10.068(-1)		
1,2-Ethanedithiol	8.96	10.54		
Ethanethiol ($\mu = 0.015$)	10.61			
Ethoxyacetic acid (18°C)	3.65			
2-Ethoxyaniline (<i>o</i> -phenetidine)	4.47(+1)			
3-Ethoxyaniline	4.17(+1)			
4-Ethoxyaniline	5.25(+1)			
2-Ethoxybenzoic acid (20°C)	4.21			
3-Ethoxybenzoic acid (20°C)	4.17			
4-Ethoxybenzoic acid (20°C)	4.80			
Ethoxycarbonylethylamine	9.13(+1)			
2-Ethoxyethanethiol	9.38			
2-Ethoxyethylamine	6.26(+1)			
2-Ethoxyphenol	10.109			
3-Ethoxyphenol	9.655			
(4-Ethoxyphenyl)phosphonic acid	2.06	7.28		
4-Ethoxypyridine	6.67(+1)			
Ethyl acetoacetate	10.68			
3-Ethylacrylic acid	4.695			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
<i>N</i> -Ethylalanine	2.22(+1)	10.22(0)		
Ethylamine	10.63(+1)			
(3-Ethylamino)phenylphosphonic				
acid	1.1(+1)	4.90(0)	7.24(-1)	
<i>N</i> -Ethylaniline	5.11(+1)			
2-Ethylaniline	4.42(+1)			
3-Ethylaniline	4.70(+1)			
4-Ethylaniline	5.00(+1)			
Ethylarsonic acid (18°C)	3.89	8.35		
Ethylbarbituric acid	3.69(+1)			
2-Ethylbenzimidazole ($\mu = 0.16$)	6.27(+1)			
2-Ethylbenzoic acid	3.79			
4-Ethylbenzoic acid	4.35			
Ethylbiguanide	2.09(+1)	11.47(0)		
2-Ethylbutanoic acid (20°C)	4.710			
S-Ethyl-L-cysteine ($\mu = 0.1$)	2.03(+1)	8.60(0)		
Ethylenebiguanide (30°C)	1.74	2.88	11.34	11.76
Ethylenebis(thioacetic acid) (18°C)	3.382(0)	4.352(-1)		
Ethylenediamine-N,N'-diacetic acid	6.42	9.46		
Ethylenediamine-N,N-dimethyl-				
N',N'-diacetic acid	6.047	10.068		
Ethylenediamine-N',N-dipropanoic				
acid (30°C)	6.87	9.60		
Ethylenediamine- <i>N</i> , <i>N</i> , <i>N</i> ′, <i>N</i> ′-				
tetraacetic acid ($\mu = 0.1$)	1.99	2.67	6.16	10.26
Ethylenediamine-N,N,N',N'-				
tetrapropanoic acid (30°C)	3.00	3.43	6.77	9.60
Ethylene glycol	14.22			
Ethyleneimine	8.04(+1)			
cis-Ethylene oxide dicarboxylic acid	1.93	3.92		
trans-Ethylene oxide dicarboxylic				
acid	1.93	3.25		
<i>N</i> -Ethylethylenediamine	7.63(+2)	10.56(+1)		
<i>N</i> -Ethylglycine ($\mu = 0.1$)	2.34(+1)	10.23(0)		
3-Ethylglutaric acid	4.28	5.33		
Ethyl hydroperoxide	11.80			
Ethyl hydrogen malonate	3.55			
3-Ethyl-2-hydroxypyridine	5.00(+1)			
Ethylmalonic acid	2.90(0)	5.55(-1)		





Ethylenebiguanide

3-Ethylglutaric acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK_3	pK_4
N-Ethyl mercaptoacetamide	8.14(SH)			
Ethyl 2-mercaptoacetate	7.95(SH)			
Ethyl 3-mercaptopropanoate	9.48(SH)			
3-Ethyl-4-(methylamino)pyridine (20°C)	9.90(+1)			
5-Ethyl-5-(1-methylbutyl)barbituric acid	8.11(0)			
Ethyl methyl ketoxime	12.45			
Ethylmethylmalonic acid	2.86(0)	6.41(-1)		
1-Ethyl-2-methylpiperidine	10.66(+1)	()		
3-Ethyl-6-methylpyridine (20°C)	6.51(+1)			
3-Ethyl-4-methylpyridine-1-oxide	-1.534(+1)			
5-Ethyl-2-methylpyridine-1-oxide	-1.288(+1)			
1-Ethyl-2-methyl-2-pyrroline	11.84(+1)			
Ethylmorphine (15 °C)	8.08			
Ethyl nitroacetate	5.85			
3-Ethylpentane-2,4-dione	11.34			
2-Ethylpentanoic acid (18°C)	4.71			
5-Ethyl-5-pentylbarbituric acid	7.960			
2-Ethylphenol	10.2			
3-Ethylphenol	10.07			
4-Ethylphenol	10.0			
4-Ethylphenylacetic acid	4.373			
5-Ethyl-5-phenylbarbituric acid	7.445			
Ethylphosphinic acid	3.29			
Ethylphosphonic acid	2.43	8.05		
1-Ethylpiperidine ($\mu = 0.01$)	10.45(+1)			
2,2-Ethylpropylglutaric acid	3.511			
Ethylpropylmalonic acid	3.14	7.43		
2-Ethylpyridine	5.89(+1)			
3-Ethylpyridine (20°C)	5.80(+1)			
4-Ethylpyridine	5.87(+1)			
Ethyl 3-pyridinecarboxylate	3.35(+1)			
Ethyl 4-pyridinecarboxylate	3.45(+1)			
2-Ethylpyridine-1-oxide	-1.19(+1)			
3-Ethylpyridine-1-oxide	-0.965(+1)			
Ethylpyrrolidine	10.43(+1)			
2-Ethyl-2-pyrroline	7.87(+1)			
Ethylsuccinic acid	4.08(0)			
S-Ethylthioacetic acid	5.06			
V-Ethyl- <i>o</i> -toluidine	4.92(+1)			
V-Ethylveratramine	7.40(+1)			
β-Eucaine	9.35(+1)			
Fluoroacetic acid	2.586			
2-Fluoroacrylic acid	2.55			
2-Fluoroaciyiic acid 2-Fluoroaniline	3.20(+1)			
z-Fluoroaniline 3-Fluoroaniline	` ′			
5-Fluoroaniline 4-Fluoroaniline	3.58(+1)			
4-Fluoroaniine 2-Fluorobenzoic acid	4.65(+1) 3.27			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-Fluorobenzoic acid	3.865			
4-Fluorobenzoic acid	4.14			
Fluoromandelic acid	4.244			
2-Fluorophenol	8.73			
3-Fluorophenol	9.29			
4-Fluorophenol	9.89			
2-Fluorophenoxyacetic acid	3.08			
3-Fluorophenoxyacetic acid	3.08			
4-Fluorophenoxyacetic acid	3.13			
4-Fluorophenylacetic acid	4.25			
2'-Fluorophenylalanine	2.14(+1)	9.01(0)		
3'-Fluorophenylalanine	2.10(+1)	8.98(0)		
4-Fluorophenylalanine	2.13(+1)	9.05(0)		
2-Fluorophenylphosphonic acid	1.64	6.80		
3-Fluorophenylselenic acid	4.34			
4-Fluorophenylselenic acid	4.50			
2-Fluoropyridine	-0.44(+1)			
3-Fluoropyridine	2.97(+1)			
5-Fluorouracil	8.00(0)	ca 13(-1)		
Folic acid (pteroylglutamic acid)	8.26	, ,		
Formic acid	3.751			
N-Formylglycine	3.43			
2-Formyl-3-hydroxypyridine (20°C)	3.40(+1)	6.95(OH)		
4-Formyl-3-hydroxypyridine	4.05(+1)	6.77(OH)		
2-Formyl-3-methoxypyridine (20°C)	3.89(+1)	12.95		
Formyl-3-methoxypyridine (20°C)	4.45(+1)	11.7		
D-(-)-Fructose	12.03			
Fumaric acid	3.10	4.60		
2-Furancarboxylic acid (2-furoic				
acid)	3.164			
D-(+)-Galactose	12.35			
Galactose-1-phosphoric acid	1.00	6.17		
Glucoascorbic acid	4.26	11.58		
D-Gluconic acid	3.86			
α -D-(+)-Glucose	12.28			
α-D-Glucose-1-phosphate	1.11(0)	6.504(-1)		
trans-Glutaconic acid	3.77	5.08		
D-(-)-Glutamic acid	2.162(+1)	4.272(0)	9.358(-1)	
L-Glutamic acid	2.13(+1)	4.31(0)	9.76(-1)	
Glutamic acid, 1-ethyl ester	3.85(+1)	7.84(0)	, ,	
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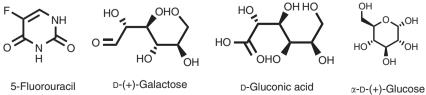


TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK ₄
Clutomic acid 5 othyd actor	2.15(+1)	9.19(0)	-	
Glutamic acid, 5-ethyl ester L-Glutamine ($\mu = 0.2$)	2.15(+1)	1 ' /		
Glutaric acid	2.15(+1) 3.77	9.00(0) 6.08		
Glutaric acid monoamide	4.600(0)	0.08		
Glutarie acid monoanide Glutarimide	11.43			
Glutathione	2.12(+1)	3.53(0)	8.66	9.12
DL-Glyceric acid	3.64	3.33(0)	8.00	9.12
Glycerol	14.15			
Glyceryl-1-phosphoric acid	14.13	6.656(-1)		
Glyceryl-2-phosphoric acid	1.335(0)	6.650(-1)		
Glycine Glycine	2.351(+1)	9.70(0)		
Glycine amide	8.03(+1)).70(0)		
Glycine, ethyl ester	7.66(+1)			
Glycine hydroxamic acid	7.10	9.10		
Glycine, methyl ester	7.59(+1)	7.10		
Glycine- <i>O</i> -phenylphosphorylserine	2.96	8.07		
Glycolic acid	3.831			
N -Glycyl- α -alanine	3.15(+1)	8.33(0)		
Glycylalanylalanine	3.38(+1)	8.10(0)		
<i>N</i> -Glycylasparagine	2.942			
Glycylaspartic acid	2.81(+1)	4.45(0)	8.60(-1)	
Glycyl-DL-glutamine (18°C)	2.88(+1)	8.33(0)	· · · · ·	
N-Glycylglycine	3.126(+1)	8.252(0)		
Glycylglycylcysteine (35°C)	2.71	2.71	7.94	7.94
Glycylglycylglycine	3.225(+1)	8.090(0)		
Glycyl-L-histidine ($\mu = 0.16$)	6.79	8.20		
Glycylisoleucine	8.00			
N-Glycyl-L-leucine	3.180(+1)	8.327(0)		
Glycyl-O-phosphorylserine	2.90	6.02	8.43	
L-Glycylproline ($\mu = 0.1$)	2.81(+1)	8.65(0)		
<i>N</i> -Glycylsarcosine ($\mu = 0.1$)	2.98(+1)	8.55(0)		
N-Glycylserine	2.98(+1)	8.38(0)		
Glycylserylglycine	3.32	7.99		
Glycyltyrosine	2.93	8.45	10.49	
Glycylvaline	3.15	8.18		
Glyoxaline	7.03(+1)			
Glyoxylic acid	3.30(0)			
Guanidineacetic acid	2.82(+1)			l

Glutaric acid

Glutathione

8.34 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Guanine	3.3(+1)	9.2	12.3	
Guanine deoxyriboside-				
3'-phosphoric acid		2.9	6.4	9.7
Guanosine	1.9(+1)	9.25(0)	12.33 (OH)	
Guanosine-5'-diphosphoric acid				
$(\mu = 0.1; pK_5 = 59.6)$			2.9	6.3
Guanosine-3'-phosphoric acid	0.7	2.3	5.92	9.38
Guanosine-5'-phosphoric acid				0.4
$(\mu = 0.1)$		2.4	6.1	9.4
Guanosine-5'-triphosphoric acid				
$[\mu = 0.1; pK_5 = 7.10(-3);$				2.0(-2)
$pK_6 = 9.3(-4)$ Guanylurea	1.80	8.20		3.0(-2)
Guanylulea	1.00	0.20		
Harmine (20°C)	7.61(+1)			
Heptafluorobutanoic acid	0.17			
4,4,5,5,6,6,6-Heptafluorohexanoic				
acid	4.18			
4,4,5,5,6,6,6-Heptafluoro-2-hexenoic				
acid	3.23			
Heptanedioic acid (pimelic acid)	4.484	5.424		
2,4-Heptanedione	8.43(keto):			
II	9.15(enol)			
Heptanoic acid Heroin	4.893			
2,4-Hexadienoic acid (sorbic	7.6(+1)			
acid)	4.77			
1,1,1,3,3,3-Hexafluoro-	7.77			
2,2-propanediol	8.801			
1,1,1,3,3,3-Hexafluoro-2-propanol	9.42			
Hexahydroazepine	11.07			
Hexamethyldisilazine	7.55			
1,2,3,8,9,10-Hexamethyl-				
4,7-phenanthroline (20°C)	7.26			
1,6-Hexanediamine	9.830(+2)	10.930(+1)		
1,6-Hexanedioic acid	4.418	5.412		
2,4-Hexanedione	8.49 (enol);			
	9.32 (keto)			
2,2',4,4',6,6'-Hexanitrodiphenylamine	5.42 (+1)			
Hexanoic acid (20°C)	4.849			
trans-2-Hexenoic acid	4.74			
trans-3-Hexenoic acid	4.72			
3-Hexen-4-oic acid	4.58			
4-Hexen-5-oic acid	4.74			
Hexylamine	10.64(+1)	0.10		
Hexylarsonic acid	4.16	9.19		
Hexylphosphonic acid DL-Histidine	2.6	7.9 6.00(+1)	9.16(0)	
DL-1118HUHIC	1.82(+2)	0.00(+1)	9.10(0)	

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK ₂	pK_3	pK_4
Histidine amide ($\mu = 0.2$)	5.78(+2)	7.64(+1)		
Histidine, methyl ester ($\mu = 0.1$)	5.01(+2)	7.23(+1)		
Histidylglycine	2.40(+2)	5.80(+1)	7.82(0)	
Histidylhistidine ($\mu = 0.16$)	5.40(+2)	6.80(+1)	7.95(0)	
DL-Homatropine	9.7(+1)			
DL-Homocysteine	2.222(+1)	8.87	10.86	
Homocysteine ($\mu = 0.1$)	1.593(+2)	2.523(+1)	8.676(0)	9.413(-1)
Hydantoin	9.12			
Hydrastine	6.23(+1)			
Hydrazine-N,N-diacetic acid	< 0.1	2.8	3.8	
Hydrazine- <i>N'</i> , <i>N'</i> -diacetic acid	2.40	3.12	7.32	
4-Hydrazinocarbonylpyridine (20°C)	1.82	3.52	10.79	
N-Hydroxyacetamide	9.40			
2'-Hydroxyacetophenone	9.90			
3'-Hydroxyacetophenone	9.19			
4'-Hydroxyacetophenone	8.05			
1-Hydroxyacridine (15°C)	5.72			
2-Hydroxyacridine (15°C)	5.62			
3-Hydroxyacridine (15°C)	5.30			
α -Hydroxyasparagine	2.28(+1)	7.20(0)		
β-Hydroxyasparagine	2.09(+1)	8.29(0)		
Hydroxyaspartic acid	1.91(+1)	3.51(0)	9.11(-1)	
2-Hydroxybenzaldehyde	, ,	` ` `		
(salicylaldehyde)	8.34			
3-Hydroxybenzaldehyde	9.00			
4-Hydroxybenzaldehyde	7.620			
2-Hydroxybenzaldehyde oxime	1.37(+1)	9.18	12.11	
2-Hydroxybenzamide	8.36			
2-Hydroxybenzenemethanol				
(2-hydroxybenzyl alcohol)	9.92			
3-Hydroxybenzenemethanol	9.83			
4-Hydroxybenzenemethanol	9.82			
4-Hydroxybenzenesulfonic acid		9.055(-1)		
2-Hydroxybenzohydroxamic acid	5.19	\ \ \ \		
2-Hydroxybenzoic acid (salicylic				
acid)	2.98	12.38		
3-Hydroxybenzoic acid	4.076	9.85		
4-Hydroxybenzoic acid	4.582	9.23		
4-Hydroxybenzonitrile	7.95			
2-Hydroxy-5-bromobenzoic acid	2.61			
2-Hydroxybutanoic acid (30°C)	3.65			

Hydantoin

8.36 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
L-3-Hydroxybutanoic acid (30°C)	4.41			
4-Hydroxybutanoic acid (30°C)	4.71			
2-Hydroxy-5-chlorobenzoic acid	2.63			
trans-2'-Hydroxycinnamic acid	4.614			
trans-3'-Hydroxycinnamic acid	4.40			
10-Hydroxycodeine	7.12			
cis-2-Hydroxycyclohexane-				
1-carboxylic acid	4.796			
trans-2-Hydroxycyclohexane-				
1-carboxylic acid	4.682			
cis-3-Hydroxycyclohexane-				
1-carboxylic acid	4.602			
trans-3-Hydroxycyclohexane-				
1-carboxylic acid	4.815			
cis-4-Hydroxycyclohexane-				
1-carboxylic acid	4.836			
trans-4-Hydroxycyclohexane-				
1-carboxylic acid	4.687			
1-Hydroxy-2,4-				
dihydroxymethylbenzene	9.79			
<i>N</i> -(Hydroxyethyl)biguanide	2.8(+2)	11.53(+1)		
<i>N</i> -(2-Hydroxyethyl)ethylenediamine	7.21(+2)	10.12(+1)		
N'-(2-Hydroxyethyl)ethylene-				
diamine-N,N,N'-triacetic acid	2.39	5.37	9.93	
<i>N</i> -(2-Hydroxyethyl)iminodiacetic				
acid ($\mu = 0.1$)	2.2	8.65		
<i>N</i> -(2-Hydroxyethyl)piperazine- <i>N</i> ′-				
ethanesulfonic acid (20°C)	7.55			
4'-(2-Hydroxyethyl)-1'-piperazine-				
propanesulfonic acid (20°C)	8.00			
2-Hydroxyethyltrimethylamine	8.94(+1)			
L-β-Hydroxyglutamic acid	2.09	4.18	9.20	
1-Hydroxy-4-hydroxymethylbenzene	9.84			
5-Hydroxy-2-(hydroxymethyl)-				
4 <i>H</i> -pyran-4-one	7.90	8.03		
3-Hydroxy-2-hydroxymethylpyridine				
$(20^{\circ}\text{C}, \mu = 0.2)$	5.00(+1)	9.07(OH)		
3-Hydroxy-4-hydroxymethylpyridine	` ′	, ,		
$(20^{\circ}\text{C}, \mu = 0.2)$	5.00(+1)	8.95(OH)		
8-Hydroxy-7-iodoquinoline-	` ′	, ,		
5-sulfonic acid	2.51(0)	7.417(-1)		
Hydroxylysine (38°C, $\mu = 0.1$)	2.13(+2)	8.62(+1)	9.67(0)	
2-Hydroxy-3-methoxybenzaldehyde	7.912	` ′	` ` ´	
3-Hydroxy-4-methoxybenzaldehyde				
(isovanillin)	8.889			
4-Hydroxy-3-methoxybenzaldehyde				
(vanillin)	7.396			
4-Hydroxy-3-methoxybenzoic acid	4.355			
1-Hydroxy-2-methoxybenzylamine	8.70(+1)	10.52(0)		

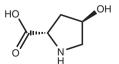
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Substance	pK ₁	pK_2	pK ₃	pK_4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2-Hydroxy-1-methoxybenzylamine	8.89(+1)	10.52(0)		
2-Hydroxy-s-methylbenzene)- methanol 2-Hydroxy-3-methylbenzoic acid 2-Hydroxy-3-methylbenzoic acid 2-Hydroxy-5-methylbenzoic acid 2-Hydroxy-5-methylbenzoic acid 2-Hydroxy-5-methylbenzoic acid 2-Hydroxy-2-methylbenzoic acid 2-Hydroxy-2-methylbutanoic acid (18°C) 3-Hydroxy-2-methylpentanoic acid (18°C) 4-Hydroxy-methylpenol 1-Hydroxymethylphenol 1-Hydroxymethylphenol 1-Hydroxy-2-methylpropanoic acid (μ=0.1) 2-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-4-methylquinoline 7-sulfonic acid 8-Hydroxy-4-methylquinoline 5-sulfonic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-4-mitrophenylphosphonic acid 2-Hydroxy-4-mitrophenzoic acid 2-Hydroxy-4-nitrobenzoic acid 2-Hydroxy-4-nitrobenzoic acid 2-Hydroxy-7-nitroduene (μ = 0.1) 4-Hydroxy-4-nitrobenzoic acid 3-Hydroxy-4-nitrobenzoic acid 3-Hydroxy-4-nitrobenzoic acid 3-Hydroxy-3-pentenicic acid 3-Hydroxy-3-pentenicic acid 3-Hydroxy-4-nitrophenpilphosphonic acid 3-Hydroxy-4-nitrophenzoic acid 3-Hydroxy-3-pentenicic acid 3-Hydroxy-4-nitrophenzoic acid 3-Hydrox					
acid 4.12 (2-Hydroxy-5-methylbenzene)-methanol 10.15 2-Hydroxy-4-methylbenzoic acid 2.99 2-Hydroxy-5-methylbenzoic acid 3.17 2-Hydroxy-5-methylbenzoic acid 4.08 2-Hydroxy-5-methylbenzoic acid 3.32 2-Hydroxy-2-methylbutanoic acid (18°C) 3-Hydroxy-2-methylputanoic acid 4.648 4-Hydroxy-4-methylpentanoic acid 4.873 1-Hydroxymethylphosphoric acid 4.873 2-Hydroxy-2-methylpropanoic acid 4.873 1-Hydroxy-4-methylpridine 4.529(+1) 8-Hydroxy-2-methylpridine 5.55(+1) 8-Hydroxy-2-methylquinoline 5.55(+1) 8-Hydroxy-2-methylquinoline-5-sulfonic acid 4.80(0) 8-Hydroxy-2-methylquinoline-5-sulfonic acid 4.78(0) 8-Hydroxy-4-methylquinoline-5-sulfonic acid 4.20(0) 8-Hydroxy-3-nitrobenzoic acid 2.23 2-Hydroxy-3-nitrobenzoic acid 2.23 2-Hydroxy-5-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-7-nitropenzoic acid 2.24 2-Hydroxy-7-nitropenzoic aci			(-)		
		4.12			
methanol 2-Hydroxy-3-methylbenzoic acid 2-Hydroxy-4-methylbenzoic acid 2-Hydroxy-5-methylbenzoic acid 3.17 2-Hydroxy-5-methylbenzoic acid 4.08 3.32 2-Hydroxy-2-methylbutanoic acid (18°C) 4.648 4.64	(2-Hydroxy-5-methylbenzene)-				
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4-Hydroxy-4-methylpentanoic acid (18°C) 1-Hydroxymethylphenol Hydroxyyethylphosphoric acid 2-Hydroxy-2-methylpropanoic acid (μ = 0.1) 2-Hydroxy-4-methylpyridine 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 5-sulfonic acid 8-Hydroxy-4-methylquinoline- 5-sulfonic acid 8-Hydroxy-1-naphthoic acid (20°C) 2-Hydroxy-1-naphthoic acid (20°C) 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-6-nitrobenzoic acid 2-Hydroxy-4-nitrophenylphosphonic acid 2-Hydroxy-7-nitroquinoline- 5-sulfonic acid 1.22 5.39 8-Hydroxy-7-nitroquinoline- 5-sulfonic acid 1.24 1.25 1.27 1.29(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 4.686 4.30 3-Hydroxy-phenylparsonic acid 3-Hydroxyphenylarsonic acid 3-Hydroxyphenylarsonic acid 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 2-Hydroxy-2-phenylpropanoic acid		1 648			
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Hydroxymethylphosphoric acid 2-Hydroxy-2-methylpropanoic acid $(μ = 0.1)$ 3.717 2-Hydroxy-4-methylpyridine 4.529(+1) 5.55(+1) 10.31(0) 8-Hydroxy-2-methylquinoline 5.55(+1) 10.00(0) 8-Hydroxy-2-methylquinoline 5.54(+1) 10.00(0) 8-Hydroxy-2-methylquinoline 4.80(0) 9.30(-1) 8-Hydroxy-4-methylquinoline-5-sulfonic acid 4.80(0) 9.30(-1) 8-Hydroxy-4-methylquinoline-5-sulfonic acid 4.20(0) 8.7(-1) 8-Hydroxy-6-methylquinoline-5-sulfonic acid 2.23 2.24 2-Hydroxy-2-nitrobenzoic acid 2.12 2.24 2-Hydroxy-3-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrophenylphosphonic acid 8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.22 5.39 8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-3-pentenoic acid 4.30 3.Hydroxyphenazine (15 °C) 4.Hydroxyphenylarsonic acid 3.Hydroxyphenylarsonic acid 3.Hydroxyphenylarsonic acid 2.Hydroxy-2-phenylpropanoic acid 3.532					
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8-Hydroxy-2-methylquinoline 8-Hydroxy-4-methylquinoline 8-Hydroxy-2-methylquinoline 8-Hydroxy-2-methylquinoline 5-sulfonic acid 4.80(0) 8-Hydroxy-4-methylquinoline 7-sulfonic acid 4.78(0) 8-Hydroxy-6-methylquinoline 5-sulfonic acid 2-Hydroxy-1-naphthoic acid (20 °C) 2-Hydroxy-1-naphthoic acid (20 °C) 2-Hydroxy-2-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-4-nitrophenylphosphonic acid 2-Hydroxy-4-nitrophenylphosphonic acid 3-Hydroxy-4-nitrotoluene (μ = 0.1) 4-Hydroxy-3-pentenoic acid 3-Hydroxy-3-pentenoic acid 3-Hydroxy-benzoic acid 3-Hydroxyphenylarsonic acid 3-Hydroxyphenylarsonic acid 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3-Hydroxyphenylboric acid 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3-Hydroxyphenylpropanoic acid 3-Hydroxyphenylpropanoic acid 3-Hydroxyp-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid 3-Hydroxy-2-phenylpropanoic acid	•				
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8-Hydroxy-2-methylquinoline-5-sulfonic acid 4.80(0) 9.30(-1) 8-Hydroxy-4-methylquinoline-7-sulfonic acid 4.78(0) 10.01(-1) 8-Hydroxy-6-methylquinoline-5-sulfonic acid 4.20(0) 8.7(-1) 2-Hydroxy-1-naphthoic acid (20 °C) 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-3-nitrobenzoic acid 2.12 2-Hydroxy-5-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrophenylphosphonic acid 2.24 8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxy-4-nitrotoluene (18 °C) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenazine (15 °C) 2.67 4-Hydroxyphenylboric acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3.532					
5-sulfonic acid 4.80(0) 9.30(-1) 8-Hydroxy-4-methylquinoline- 4.78(0) 10.01(-1) 8-Hydroxy-6-methylquinoline- 4.20(0) 8.7(-1) 5-sulfonic acid 4.20(0) 8.7(-1) 2-Hydroxy-1-naphthoic acid (20°C) 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-3-nitrobenzoic acid 1.87 2-Hydroxy-5-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrophenylphosphonic acid 1.22 3-Hydroxy-7-nitroquinoline- 5-sulfonic acid 5-sulfonic acid 1.94(0) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenazine (15°C) 2.67 4-Hydroxyphenylarsonic acid 8.55 3-Hydroxyphenylboric acid 8.55 2-Hydroxy-2-phenylpropanoic acid 3.532		3.30(+1)	10.00(0)		
8-Hydroxy-4-methylquinoline-7-sulfonic acid 4.78(0) 10.01(-1) 8-Hydroxy-6-methylquinoline-5-sulfonic acid 4.20(0) 8.7(-1) 2-Hydroxy-1-naphthoic acid (20 °C) 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-5-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrophenylphosphonic acid 1.22 5.39 8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxy-henzine (15 °C) 4-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3.532		4.90(0)	0.20(1)		
7-sulfonic acid 4.78(0) $10.01(-1)$ 8-Hydroxy-6-methylquinoline-5-sulfonic acid 4.20(0) 8.7(-1) 2-Hydroxy-1-naphthoic acid (20 °C) 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-5-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.12 2-Hydroxy-4-nitrophenylphosphonic acid 1.22 3-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 3-Hydroxy-4-nitrotoluene ($μ = 0.1$) 7.41 4-Hydroxy-9-pentanoic acid (18 °C) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 8.55 2-Hydroxy-2-phenylpropanoic acid 3.532		4.80(0)	9.30(-1)		
8-Hydroxy-6-methylquinoline-5-sulfonic acid $4.20(0)$ 3.29 9.68 $2-Hydroxy-1-naphthoic acid 20^{\circ}\text{C} 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-3-nitrobenzoic acid 2.12 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-6-nitrobenzoic acid 2.24 2-Hydroxy-4-nitrophenylphosphonic acid 2.24 2-Hydroxy-7-nitroquinoline-5-sulfonic acid 2.12 2-Hydroxy-4-nitrotoluene (\mu=0.1) 2-Hydroxy-3-pentenoic acid 3-Hydroxy-3-pentenoic acid 3-Hydroxy-3-penteno$		4.70(0)	10.01(1)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		4.78(0)	10.01(-1)		
2-Hydroxy-1-naphthoic acid (20°C) 3.29 9.68 2-Hydroxy-2-nitrobenzoic acid 2.23 2-Hydroxy-3-nitrobenzoic acid 2.Hydroxy-5-nitrobenzoic acid 2-Hydroxy-6-nitrobenzoic acid 2-Hydroxy-4-nitrophenylphosphonic acid 2-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.22 5.39 3-Hydroxy-4-nitrotoluene (μ = 0.1) 4.Hydroxy-4nitrotoluene (μ = 0.1) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenzine (15°C) 2.67 4-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3.532		4.20(0)	0.7(1)		
2-Hydroxy-2-nitrobenzoic acid 2-Hydroxy-3-nitrobenzoic acid 2-Hydroxy-5-nitrobenzoic acid 2-Hydroxy-6-nitrobenzoic acid 2-Hydroxy-6-nitrobenzoic acid 2-Hydroxy-4-nitrophenylphosphonic acid 1.22 5.39 8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 4.14 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenzine (15°C) 2.67 4-Hydroxyphenzine (15°C) 2.67 4-Hydroxyphenylboric acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3.532		` ′			
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8-Hydroxy-7-nitroquinoline-5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxypentanoic acid (18 °C) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenazine (15 °C) 2.67 4-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532		4.00			
5-sulfonic acid 1.94(0) 5.750(-1) 3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxypentanoic acid (18°C) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 8.55 2-Hydroxy-2-phenylpropanoic acid 3.532		1.22	5.39		
3-Hydroxy-4-nitrotoluene (μ = 0.1) 7.41 4-Hydroxypentanoic acid (18 °C) 4.686 4-Hydroxy-3-pentenoic acid 4.30 3-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532					
4-Hydroxypentanoic acid (18°C) 4-Hydroxy-3-pentenoic acid 3-Hydroxyphenazine (15°C) 2-67 4-Hydroxyphenylarsonic acid 3-Hydroxyphenylboric acid 3-Hydroxyphenylboric acid 8-55 10.84 2-Hydroxy-2-phenylpropanoic acid 3-532		\ /	5.750(-1)		
4-Hydroxy-3-pentenoic acid 3-Hydroxyphenazine (15 °C) 2.67 4-Hydroxyphenylarsonic acid 3-Hydroxyphenylboric acid 3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532	3-Hydroxy-4-nitrotoluene ($\mu = 0.1$)				
3-Hydroxyphenazine (15 °C) 4-Hydroxyphenylarsonic acid 3-Hydroxyphenylboric acid 3-Hydroxyphenylboric acid 2-Hydroxy-2-phenylpropanoic acid 3.532					
4-Hydroxyphenylarsonic acid 3.89 8.37 10.05 (phenol) 3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532					
3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532					
3-Hydroxyphenylboric acid 8.55 10.84 2-Hydroxy-2-phenylpropanoic acid 3.532	4-Hydroxyphenylarsonic acid	3.89	8.37		
2-Hydroxy-2-phenylpropanoic acid 3.532	3-Hydroxyphenylboric acid	8.55	10.84	u ,	
2-(2-Hydroxyphenyl)pyridine (20°C) 4.19(±1) 10.64	2-(2-Hydroxyphenyl)pyridine (20°C)	4.19(+1)	10.64		

8.38 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK_4
trans-4-Hydroxyproline	1.818(+1)	9.662(0)		
Hydroxypropanedioic acid (tartronic				
acid)	2.37	4.74		
2-Hydroxypropanoic acid	3.858			
1-Hydroxy-2-propylbenzene	10.50			
4-Hydroxypteridine	1.3(+1)	7.89(0)		
2-Hydroxypyridine	1.25(+1)	11.62(0)		
3-Hydroxypyridine	4.80(+1)	8.72(0)		
4-Hydroxypyridine	3.23(+1)	11.09(0)		
2-Hydroxypyridine-N-oxide	-0.62(+1)	5.97(0)		
2-Hydroxypyrimidine	2.24(+1)	9.17(0)		
4-Hydroxypyrimidine	1.85(+1)	8.59(0)		
8-Hydroxyquinazoline	3.41(+1)	8.65(0)		
2-Hydroxyquinoline (20°C)	-0.31(+1)	11.74		
3-Hydroxyquinoline (20°C)	4.30(+1)	8.06(0)		
4-Hydroxyquinoline (20°C)	2.27(+1)	11.25(0)		
5-Hydroxyquinoline (20°C)	5.20(+1)	8.54(0)		
6-Hydroxyquinoline (20°C)	5.17(+1)	8.88(0)		
7-Hydroxyquinoline (20°C)	5.48(+1)	8.85(0)		
8-Hydroxyquinoline (20°C)	4.91(+1)	9.81(0)		
8-Hydroxyquinoline-5-sulfonic acid	4.092(+1)	8.776(0)		
DL-Hydroxysuccinic acid (malic acid)	3.458	5.097		
L-Hydroxysuccinic acid	3.40	5.05		
Hydroxytetracycline	3.27(+1)	7.32(0)	9.11(-1)	
5-Hydroxy-1,2,3,4-tetrazole	3.32			
4-Hydroxy-3-(2'-thiazolyazo)toluene	8.36			
2-Hydroxytoluene	10.33			
3-Hydroxytoluene	10.10			
4-Hydroxytoluene	10.276			
4-Hydroxy- α , α , α -trifluorotoluene	8.675			
1-Hydroxy-2,4,6-				
trihydroxymethylbenzene	9.56			
Hydroxyuracil	8.64			
Hydroxyvaline	2.55(+1)	9.77(0)		
Hyoscyamine	9.68(+1)			
Hypoxanthene	1.79(+1)	8.91(0)	12.07(-1)	
Hypoxanthine	5.3			
Imidazole	6.993(+1)	10.58(0)		
Imidazolidinetrione (parabanic acid)	6.10			





Imidazole

trans-4-Hydroxyproline

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

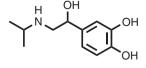
Substance	pK_1	pK_2	pK_3	pK_4
4-(4-Imidazolyl)butanoic acid				
$(\mu = 0.1)$	4.26(+1)	7.62(0)		
2-(4-Imidazolyl)ethylamine	5.784(+2)	9.756(+1)		
3-(4-Imidazolyl)propanoic acid				
$(\mu = 0.16)$	3.96(+1)	7.57(0)		
3,3'-Iminobispropanoic acid	4.11(0)	9.61(-1)		
3,3'-Iminobispropylamine (30°C)	8.02(+2)	9.70(+1)	10.70(0)	
2,2'-Iminodiacetic acid (diglycine)				
$(30^{\circ}\text{C}, \mu = 0.1)$	2.54(0)	9.12(-1)		
4-Indanol	10.32			
Indole-3-acetic acid	4.75			
Inosine	ca 1.5(+1)	8.96(0)	12.36	
Inosine-5'-phosphoric acid	1.54(0)	6.66(-1)		
Inosine-5'-triphosphoric acid				
$[pK_5 = 7.68(-4)]$			2.2(-2)	6.92(-3)
Iodoacetic acid	3.175			
2-Iodoaniline	2.54(+1)			
3-Iodoaniline	3.58(+1)			
4-Iodoaniline	3.82(+1)			
2-Iodobenzoic acid	2.86			
3-Iodobenzoic acid	3.86			
4-Iodobenzoic acid	4.00			
5-Iodohistamine	4.06(+2)	9.20(+1)	11.88(0)	
	(imidazole)	(NH_3^+)	(imino)	
7-Iodo-8-hydroxyquinoline-5-sulfonic		-		
acid	2.514	7.417		
Iodomandelic acid	3.264			
Iodomethylphosphoric acid	1.30	6.72		
2-Iodophenol	8.464			
3-Iodophenol	8.879			
4-Iodophenol	9.200			
2-Iodophenoxyacetic acid	3.17			
3-Iodophenoxyacetic acid	3.13			
4-Iodophenoxyacetic acid	3.16			
2-Iodophenylacetic acid	4.038			
3-Iodophenylacetic acid	4.159			
4-Iodophenylacetic acid	4.178			
2-Iodophenylphosphoric acid	1.74	7.06		
2-Iodopropanoic acid	3.11			
3-Iodopropanoic acid	4.08			
2-Iodopyridine	1.82(+1)			

Inosine

8.40 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK_3	pK_4
3-Iodopyridine	3.25(+1)			
4-Iodopyridine (20°C)	4.02(+1)			
Isoasparagine	2.97(+1)	8.02(0)		
Isobutylacetic acid (18°C)	4.79	` ′		
Isobutylamine	10.41(+1)			
Isochlorotetracycline	3.1(+1)	6.7(0)	8.3(-1)	
Isocreatine	2.84(+1)			
Isoglutamine	3.81(+1)	7.88(0)		
Isohistamine ($\mu = 0.1$)	6.036(+2)	9.274(+1)		
L-Isoleucine	2.318(+1)	9.758(0)		
Isolysergic acid	3.33(0)	8.46(NH)		
Isopilocarpine (15°C)	7.18(+1)			
2-(Isopropoxy)benzoic acid (20°C)	4.24			
3-(Isopropoxy)benzoic acid (20°C)	4.15			
4-(Isopropoxy)benzoic acid (20°C)	4.68			
Isopropylamine	10.64(+1)			
N-Isopropylaniline	5.50(+1)			
5-Isopropylbarbituric acid	4.907(+1)			
2-Isopropylbenzene acid	3.64			
4-Isopropylbenzoic acid	4.36			
<i>N</i> -Isopropylglycine ($\mu = 0.1$)	2.36(+1)	10.06(0)		
Isopropylmalonic acid	2.94	5.88		
Isopropylmalonic acid mononitrile	2.401			
3-Isopropyl-4-(methylamino)pyridine				
(20°C)	9.96(+1)			
3-Isopropylpentanedioic acid	4.30	5.51		
4-Isopropylphenylacetic acid	4.391			
Isopropylphosphinic acid	3.56			
Isopropylphosphonic acid	2.66	8.44		
2-Isopropylpyridine	5.83(+1)			
3-Isopropylpyridine (20°C)	5.72(+1)			
4-Isopropylpyridine	6.02(+1)			
DL-Isoproterenol	8.64(+1)			
Isoquinoline	5.40(+1)			
Isoretronecanol	10.83			
L-Isoserine ($\mu = 0.16$)	2.72(+1)	9.25(0)		
Isothiocyanatoacetic acid	6.62			
L-(+)-Lactic acid	3.858			
L-Leucine	2.328(+1)	9.744(0)		
Leucine amide	7.80(+1)			



N N OH

DL-Isoproterenol

Isoquinoline

Isoretronecanol

TABLE 8.1 pK_A Values of Organic Materials in Water at 25° C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Leucine, ethyl ester ($\mu = 0.1$)	7.57(+1)			
L-Leucyl-L-asparagine	3.00(+1)	8.12(0)		
L-Leucyl-L-glutamine	2.99(+1)	8.11(0)		
DL-Leucylglycine	3.25(+1)	8.28(0)		
Leucylisoserine (20°C)	3.188(+1)	8.207(0)		
D-Leucyl-L-tyrosine	3.12(+1)	8.38(0)	10.35(-1)	
L-Leucyl-L-tyrosine	3.46(+1)	7.84(0)	10.09(-1)	
Lysergic acid	3.44(+1)	7.68(0)		
L-(+)-Lysine	2.18(+2)	8.95(+1)	10.53(0)	
Lysine, methyl ester ($\mu = 0.1$)	6.965(+1)	10.251(0)		
L-Lysyl-L-alanine	3.22(+1)	7.62(0)	10.70(-1)	
L-Lysyl-D-alanine	3.00(+1)	7.74(0)	10.63(-1)	
Lysylglutamic acid	2.93(+2)	4.47(+1)	7.75(0)	10.50(+1)
L-Lysyl-L-lysine ($\mu = 0.1$)	3.01(+2)	7.53(+1)	10.05(0)	10.01(-1)
L-Lysyl-D-lysine ($\mu = 0.1$)	2.85(+2)	7.53(+1)	9.92(0)	10.89(-1)
L-Lysyl-L-lysyle ($\mu = 0.1$)	3.08(+2)	7.34(+1)	9.80(0)	10.54(-1)
L-Lysyl-D-lysyl-L-lysine ($\mu = 0.1$)	2.91(+2)	7.29(+1)	9.79(0)	10.54(-1)
L-Lysyl-D-lysyl-lysine ($\mu = 0.1$)	2.94(+2)	7.15(+1)	9.60(0)	10.38(-1)
α-D-Lyxose	12.11			
Maleic acid	1.910	6.33		
Malonamic acid	3.641(0)			
Malonic acid	2.826	5.696		
Malonitrile (cyanoacetic acid)	2.460			
Mandelic acid	3.411			
D-(+)-Mannose	12.08			
Mercaptoacetic acid (thioglycolic				
acid)	3.60(0)	10.56(SH)		
2-Mercaptobenzoic acid (20°C)	4.05(0)			
2-Mercaptobutanoic acid	3.53(0)			
Mercaptodiacetic acid	3.32	4.29		
2-Mercaptoethanesulfonic acid (20°C)		9.5(-1)		
2-Mercaptoethanol	9.88			
2-Mercaptoethylamine	8.27(+1)	10.53(0)		
2-Mercaptohistidine	1.84(+1)	8.47(0)	11.4(SH)	
Mercapto-S-phenylacetic acid				
$(\mu = 0.1)$	3.9			
2-Mercaptopropane ($\mu = 0.1$)	10.86			
3-Mercapto-1,2-propanediol ($\mu = 0.5$)	9.43			
2-Mercaptopropanoic acid	4.32(0)	10.20(SH)		
3-Mercaptopropanoic acid		10.84(SH)		

Mandelic acid

D-(+)-Mannose

8.42 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK ₃	pK_4
2-Mercaptopyridine (20°C)	-1.07(+1)	10.00(0)		
3-Mercaptopyridine (20°C)	2.26(+1)	7.03(0)		
4-Mercaptopyridine (20°C)	1.43(+1)	8.86(0)		
2-Mercaptoquinoline (20°C)	-1.44(+1)	10.21(0)		
3-Mercaptoquinoline (20°C)	2.33(+1)	6.13(0)		
4-Mercaptoquinoline (20°C)	0.77(+1)	8.83(0)		
Mercaptosuccinic acid	3.30(0)	4.94(-1)	10.94(SH)	
Mesitylenic acid	4.32			
Mesoxaldialdehyde	3.60			
Methacrylic acid	4.66			
Methanethiol	10.70			
DL-Methionine	2.13(+1)	9.28(0)		
2-(N-Methoxyacetamido)pyridine	2.01(+1)			
3-(N-Methoxyacetamido)pyridine	3.52(+1)			
4-(N-Methoxyacetamido)pyridine	4.62(+1)			
Methoxyacetic acid	3.570			
3-Methoxy-D- α -alanine	2.037(+1)	9.176(0)		
2-Methoxyaniline	4.53(+1)			
3-Methoxyaniline	4.20(+1)			
4-Methoxyaniline	5.36(+1)			
2-Methoxybenzoic acid	4.09			
3-Methoxybenzoic acid	4.08			
4-Methoxybenzoic acid	4.49			
N,N-Methoxybenzylamine	9.68(+1)			
2-Methoxycarbonylaniline	2.23(+1)			
3-Methoxycarbonylaniline	3.64(+1)			
4-Methoxycarbonylaniline	2.38(+1)			
Methoxycarbonylmethylamine	7.66(+1)			
2-Methoxycarbonylpyridine	2.21(+1)			
3-Methoxycarbonylpyridine	3.13(+1)			
4-Methoxycarbonylpyridine	3.26(+1)			
trans-2-Methoxycinnamic acid	4.462			
trans-3-Methoxycinnamic acid	4.376			
trans-4-Methoxycinnamic acid	4.539			
2-Methoxyethylamine	9.45(+1)			
2-Methoxy-4-nitrophenylphosphonic				
acid	1.53	6.96		
2-Methoxyphenol	9.99			
3-Methoxyphenol	9.652			
4-Methoxyphenol	10.20			
(2'-Methoxy)phenoxyacetic acid	3.231			



Mesitylenic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK_4
(3'-Methoxy)phenoxyacetic acid	3.141			
(4'-Methoxy)phenoxyacetic acid	3.213			
4'-Methoxyphenylacetic acid	4.358			
(4-Methoxyphenyl)phosphinic acid				
(17°C)	2.35			
2-Methoxyphenyl)phosphonic acid	2.16	7.77		
4-Methoxyphenyl)phosphonic acid				
(17°C)	2.4	7.15		
3-(2'-Methoxyphenyl)propanoic acid	4.804			
-(3'-Methoxyphenyl)propanoic acid	4.654			
3-(4'-Methoxyphenyl)propanoic acid	4.689			
3-Methoxyphenylselenic acid	4.65			
-Methoxyphenylselenic acid	5.05			
2-Methoxy-4-(2-propenyl)phenol	10.0			
-Methoxypyridine	3.06(+1)			
3-Methoxypyridine	4.91(+1)			
-Methoxypyridine	6.47(+1)			
-Methoxy-2-(2'-thiazoylazo)phenol	7.83			
-Methylacrylic acid (18°C)	4.66			
V-Methylalanine	2.22(+1)	10.19(0)		
O-Methylallothreonine ($\mu = 0.1$)	1.92(+1)	8.90(0)		
Methylamine	10.62(+1)			
2-(N-Methylamino)benzoic acid	1.93(+1)	5.34(0)		
3-(<i>N</i> -Methylamino)benzoic acid		5.10(0)		
-(N-Methylamino)benzoic acid		5.05		
Methylaminodiacetic acid (20°C)	2.146	10.088		
2-(Methylamino)ethanol	9.88(+1)			
2-(2-Methylaminoethyl)pyridine				
(30°C)	3.58(+2)	9.65(+1)		
2-(Methylaminomethyl)-6-methyl-		,		
pyridine				
$(\mu = 0.5)$	3.03(+2)	9.15(+1)		
2-(Methylaminomethyl)pyridine				
(30°C)	2.92(+2)	8.82(+1)		
l-Methylamino-3-methylpyridine				
(20°C)	9.83(+1)			
3-Methylamino)phenylphosphonic	` ´			
acid	1.1(+1)	4.72(+1)	7.30(-1)	
4-Methylamino)phenylphosphonic				
acid			7.85(-1)	
-(Methylamino)pyridine (30°C)	8.70(+1)			
-(Methylamino)pyridine (20°C)	9.65(+1)			
-(Methylamino)-2,3,5,6-tetramethyl-				
pyridine (20°C)	10.06(+1)			
V-Methylaniline	4.85(+1)			
Methylarsonic acid (18°C)	3.41	8.18		
-Methylbarbituric acid	4.35(+1)	0.10		
5-Methylbarbituric acid	3.386(+1)			
2-(<i>N</i> -Methylbenzamido)pyridine	1.44(+1)			
2 (2) Michigipenzamido/pyridine	1.77(1)			

8.44 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-(<i>N</i> -Methylbenzamido)pyridine	3.66(+1)			
4-(<i>N</i> -Methylbenzamido)pyridine	4.68(+1)			
2-Methylbenzimidazole ($\mu = 0.16$)	6.29(+1)			
2-Methylbenzoic acid (<i>o</i> -toluic acid)	3.90			
3-Methylbenzoic acid	4.269			
4-Methylbenzoic acid	4.362			
<i>N</i> -Methyl-1-benzoylecgonine	8.65			
Methylbiguanidine	3.00(+2)	11.44(+1)		
2-Methyl-2-butanethiol	11.35	, ,		
2-Methylbutanoic acid	4.761			
3-Methylbutanoic acid (20°C)	4.767			
(E)-2-Methyl-2-butendioic acid				
(mesaconic acid)	3.09	4.75		
3-Methyl-2-butenoic acid	5.12			
(E)-2-Methyl-2-butenoic acid				
(tiglic acid)	4.96			
(Z)-2-Methyl-2-butenoic acid				
(angelic acid)	4.30			
4-Methylcarboxylphenol	8.47			
(<i>E</i>)-2-Methylcinnamic acid	4.500			
(E)-3-Methylcinnamic acid	4.442			
(E)-4-Methylcinnamic acid	4.564			
1-Methylcyclohexane-1-carboxylic				
acid	5.13			
cis-2-Methylcyclohexane-	0.10			
1-carboxylic acid	5.03			
trans-2-methylcyclohexane-				
1-carboxylic acid	5.73			
cis-3-methylcyclohexane-				
1-carboxylic acid	4.88			
trans-3-Methylcyclohexane-				
1-carboxylic acid	5.02			
cis-4-Methylcyclohexane-	5.02			
1-carboxylic acid	5.04			
trans-4-Methylcyclohexane-	5.0.			
1-carboxylic acid	4.89			
2-Methylcyclohexyl-1,1-diacetic acid	3.53	6.89		
3-Methylcyclohexyl-1,1-diacetic acid	3.49	6.08		
4-Methylcyclohexyl-1,1,1-diacetic	3.17	0.00		
acid	3.49	6.10		
3-Methylcyclopentyl-1,1-diacetic acid	3.79	6.74		
S-Methyl-L-cysteine	8.97	0.71		
<i>N</i> -Methylcytidine	3.88			
5-Methylcytidine	4.21			
<i>N</i> -Methyl-2'-deoxycytidine	3.97			
5-Methyl-2'-deoxycytidine	4.33			
2-Methyl-3,5-dinitrobenzoic acid	2.97			
5-Methyldipropylenetriamine (30°C)	6.32(+3)	9.19(+2)	10.33(+1)	
2,2'-Methylenebis(4-chlorophenol)	7.6	9.19(+2)	10.55(±1)	
2,2 Methyleneois(4-emotophenoi)	7.0	11.5		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK ₃	pK_4
2,2'-Methylenebis(4,6-dichloro-				
phenol)	5.6	10.56		
Methylenebis(thioacetic acid) (18°C)	3.310	4.345		
3,3'-(Methylenedithio)dialanine	2.200(+1)	8.16(0)		
Methylenesuccinic acid	3.85	5.45		
<i>N</i> -Methylethylamine	4.23(+1)			
N-Methylethylenediamine	6.86(+1)	10.15(+1)		
α -Methylglucoside	13.71	\ \ \ \ \ \		
3-Methylglutaric acid	4.24	5.41		
N-Methylglycine (sarcosine)	2.12(+1)	10.20(0)		
5-Methyl-2,4-heptanedione	8.52(enol); 9.10(keto)			
5-Methyl-2,4-hexanedione	8.66(enol); 9.31(keto)			
5-Methyl-4-hexenoic acid	4.80			
3-Methylhistamine	5.80(+1)	9.90(0)		
1-Methylhistidine	1.69	6.48	8.85	
2-Methylhistidine (18 °C)	1.7	7.2	9.5	
2-Methyl-8-hydroxyquinoline			- 10	
$(\mu = 0.005)$	4.58(+1)	11.71(0)		
4-Methyl-8-hydroxyquinoline	4.67(+1)	11.62(0)		
1-Methylimidazole	7.06(+1)			
4-Methylimidazole	7.55(+1)			
N-Methyliminodiacetic acid	2.15	10.09		
S-Methylisothiourea	9.83(+1)			
O-Methylisourea	9.72(+1)			
Methylmalonic acid	3.07	5.87		
2-(N-Methylmethane-				
sulfonamido)pyridine	1.73(+1)			
3-(<i>N</i> -Methylmethane-				
sulfonamido)pyridine	3.94(+1)			
4-(<i>N</i> -Methylmethane-	0.5.(. 1)			
sulfonamido)pyridine	5.14(+1)			
2-Methyl-6-methyl-	0.1.(. 1)			
aminopyridine (20°C)	3.17(+1)	8.84(0)		
3-Methyl-4-methyl-	3117(11)	0.0.(0)		
aminopyridine (20°C)		9.84(0)		
4-Methyl-2,2'-		7.01(0)		
(4-methylpyridyl)pyridine	5.32(+1)			
N-Methylmorpholine	7.13(+1)			
2-Methyl-1-naphthoic acid	3.11			
N-Methyl-1-naphthylamine	3.70(+1)			
2-Methyl-4-nitrobenzoic acid	1.86			
2-Methyl-6-nitrobenzoic acid	1.87			
1-Methyl-2-nitroterephthalic acid	3.11			
4-Methyl-2-nitroterephthalic acid	1.82			
3-Methylpentanedioic acid	4.25	5.41		
3-Methylpentane-2,4-dione	10.87	J.71		
2-Methylpentanoic acid	4.782			
2-iviemy ipentanoie actu	4.702			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK_3	pK_4
3-Methylpentanoic acid	4.766			
4-Methylpentanoic acid	4.845			
cis-3-Methyl-2-pentenoic acid	5.15			
trans-3-Methyl-2-pentenoic acid	5.13			
4-Methyl-2-pentenoic acid	4.70			
4-Methyl-3-pentenoic acid	4.60			
6-Methyl-1,10-phenanthroline	5.11(+1)			
(2-Methylphenoxy)acetic acid	3.227			
(3-Methylphenoxy)acetic acid	3.203			
(4-Methylphenoxy)acetic acid	3.215			
(2-Methylphenyl)acetic acid (18°C)	4.35			
(4-Methylphenyl)acetic acid	4.370			
5-Methyl-5-phenylbarbituric acid	8.011(0)			
3-(2-Methylphenyl)propanoic acid	4.66			
3-(3-Methylphenyl)propanoic acid	4.677			
3-(4-Methylphenyl)propanoic acid	4.684			
1-Methyl-2-phenylpyrrolidine	8.80			
5-Methyl-1-phenyl-1,2,3-triazole-				
4-carboxylic acid	3.73			
Methylphosphinic acid	3.08			
Methylphosphonic acid	2.38	7.74		
3-Methyl-o-phthalic acid	3.18			
4-Methyl-o-phthalic acid	3.89			
<i>N</i> -Methylpiperazine ($\mu = 0.1$)	4.94(+2)	9.09(+1)		
2-Methylpiperazine	5.62(+2)	9.60(+1)		
N-Methylpiperidine	10.19(+1)			
2-Methylpiperidine	10.95(+1)			
3-Methylpiperidine	11.07(+1)			
4-Methylpiperidine ($\mu = 0.5$)	11.23(+1)			
2-Methyl-1,2-propanediamine	6.178(+2)	9.420(+1)		
2-Methyl-2-propanethiol	11.2			
2-Methylpropanoic acid	4.853			
2-Methyl-2-propylamine	10.682(+1)			
2-Methyl-2-propylglutaric acid	3.626			
2-Methylpyridine	5.96(+1)			
3-Methylpyridine	5.68(+1)			
4-Methylpyridine	6.00(+1)			
Methyl 4-pyridinecarboxylate	3.26(+1)			
6-Methylpyridine-2-carboxylic acid	5.83			
2-Methylpyridine-1-oxide	1.029(+1)			
3-Methylpyridine-1-oxide	10.921(+1)			
4-Methylpyridine-1-oxide	1.258(+1)			
<i>O</i> -Methylpyridoxal ($\mu = 0.16$)	4.74			
Methyl-2-pyridyl ketoxime	9.97			
1-Methyl-2-(3-pyridyl)pyrrolidine	3.41	7.94		
1-Methylpyrrolidine	10.46(+1)			
1-Methyl-3-pyrroline	9.88(+1)			
5-Methylquinoline	4.62(+1)			
Methylsuccinic acid	4.13	5.64		
Methylsulfonylacetic acid	2.36			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK ₃	pK ₄
3-Methylsulfonylaniline	2.68(+1)			
4-Methylsulfonylaniline	1.48(+1)			
3-Methylsulfonylbenzoic acid	3.52			
4-Methylsulfonylbenzoic acid	3.64			
4-Methylsulfonyl-3,5-dimethylphenol	8.13			
3-Methylsulfonylphenol	9.33			
4-Methylsulfonylphenol	7.83			
1-Methyl-1,2,3,4-tetrahydro-				
3-pyridinecarboxylic acid				
(arecaidine; isoguvacine)	9.07			
5-Methyl-1,2,3,4-tetrazole	3.32			
2-Methylthiazole ($\mu = 0.1$)	3.40(+1)			
4-Methylthiazole ($\mu = 0.1$)	3.16(+1)			
5-Methylthiazole ($\mu = 0.1$)	3.03(+1)			
Methylthioacetic acid	3.72			
1-Methylthioaniline	4.40(+1)			
2-Methylthioethylamine (30°C)	9.18(+1)			
Methylthioglycolic acid	7.68			
3-(S-Methylthio)phenol	9.53			
1-(S-Methylthio)phenol	9.53			
2-Methylthiopyridine (20°C)	3.59(+1)			
3-Methylthiopyridine (20°C)	4.42(+1)			
1-Methylthiopyridine (20°C)	5.94(+1)			
5-Methylthio-1,2,3,4-tetrazole	4.00(+1)			
O-Methylthreonine	2.02(+1)	9.00(0)		
O-Methyltyrosine	2.21(+1)	9.35(0)		
l-Methylxanthine	7.70	12.0		
3-Methylxanthine	8.10	11.3		
7-Methylxanthine	8.33	ca 13		
9-Methylxanthine	6.25			
Morphine (20°C)	7.87(+1)	9.85(0)		
Morpholine	8.492(+1)			
2-(<i>N</i> -Morpholino)ethanesulfonic				
acid (MES) (20°C)	6.15			
3-(N-Morpholino)-2-hydroxy-				
propanesulfonic acid (37°C)	6.75			
3-(N-Morpholino)propanesulfonic				
acid (20°C)	7.20			
Murexide	0.0	9.20	10.50	
Myosmine	5.26			
1-Naphthalenecarboxylic acid				
(1-naphthoic acid)	3.695			
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Morpholine

Myosmine

1-Naphthalenecarboxylic acid

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK ₄
2-Naphthalenecarboxylic acid	4.161			
1-Naphthol (20°C)	9.30			
2-Naphthol (20°C)	9.57			
Naphthoquinone monoxime	8.01			
1-Naphthylacetic acid	4.236			
2-Naphthylacetic acid	4.256			
1-Naphthylamine	3.92(+1)			
2-Naphthylamine	4.11(+1)			
1-Naphthylarsonic acid	3.66	8.66		
1-Naphthylsulfonic acid	0.57			
Narceine (15°C)	3.5(+1)	9.3		
Narcotine	6.18(+1)			
Nicotine	3.15(+1)	7.87(0)		
Nicotyrine	4.76(+1)			
Nitrilotriacetic acid (NTA) (20°C)	1.65	2.94	10.33	
Nitroacetic acid	1.68			
2-Nitroaniline	-0.28(+1)			
3-Nitroaniline	2.46(+1)			
4-Nitroaniline	1.01(+1)			
2-Nitrobenzene-1,4-dicarboxylic acid	1.73			
3-Nitrobenzene-1,2-dicarboxylic acid	1.88			
4-Nitrobenzene-1,2-dicarboxylic acid	2.11			
2-Nitrobenzoic acid	2.18			
3-Nitrobenzoic acid	3.46			
4-Nitrobenzoic acid	3.441			
trans-2-Nitrocinnamic acid	4.15			
trans-3-Nitrocinnamic acid	4.12			
trans-4-Nitrocinnamic acid	4.05			
Nitroethane	8.57			
2-Nitrohydroquinone	7.63	10.06		
N-Nitroiminodiacetic acid	2.21	3.33		
3-Nitromesitol	8.984			
Nitromethane	10.21			
1-Nitro-6,7-phenanthroline ($\mu = 0.2$)	3.23(+1)			
5-Nitro-1,10-phenanthroline	3.232(+1)			
6-Nitro-1,10-phenanthroline	3.23(+1)			
2-Nitrophenol	7.222			
3-Nitrophenol	8.360			
4-Nitrophenol	7.150			
(2-Nitrophenoxy)acetic acid	2.896			

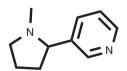


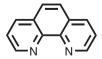
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK_3	pK_4
(3-Nitrophenoxy)acetic acid	2.951			
(4-Nitrophenoxy)acetic acid	2.893			
2-Nitrophenylacetic acid	4.00			
3-Nitrophenylacetic acid	3.97			
4-Nitrophenylacetic acid	3.85			
2-Nitrophenylarsonic acid	3.37	8.54		
3-Nitrophenylarsonic acid	3.41	7.80		
4-Nitrophenylarsonic acid	2.90	7.80		
7-(4-Nitrophenylazo)-8-hydroxy-				
5-quinolinesulfonic acid	3.14(0)	7.495(-1)		
3-Nitrophenylphosphonic acid	1.30	6.27		
4-Nitrophenylphosphonic acid	1.24	6.23		
3-(2'-Nitrophenyl)propanoic acid	4.504			
3-(4'-Nitrophenyl)propanoic acid	4.473			
3-Nitrophenylselenic acid	4.07			
4-Nitrophenylselenic acid	4.00			
1-Nitropropane	8.98			
2-Nitropropane	7.675			
2-Nitropropanoic acid	3.79			
2-Nitropyridine ($\mu = 0.02$)	-2.06(+1)			
3-Nitropyridine ($\mu = 0.02$)	0.79(+1)			
4-Nitropyridine ($\mu = 0.02$)	1.23(+1)			
N-Nitrosoiminodiacetic acid	2.28	3.38		
4-Nitrosophenol	6.48			
Nitrourea	4.15(+1)			
1,9-Nonanedioic acid (azelaic acid)	4.53	5.40		
Nonanoic acid (pelargonic acid)	4.95			
DL-Norleucine	2.335(+1)	9.834(0)		
Novocaine	8.85(+1)			
2,2,3,3,4,4,5,5-Octafluoropentanoic				
acid	2.65			
1,8-Octanedioic acid (suberic acid)	4.512	5.404		
Octanoic acid (caprylic acid)	4.895			
Octopine-DD	1.35	2.30	8.68	11.25
Octopine-LD	1.40	2.30	8.72	11.34
Octylamine	10.65(+1)	0.65(1.4)	10.5(0)	
L-(+)-Ornithine	1.94(+2)	8.65(+1)	10.76(0)	
Oxalic acid	1.271	4.272		
3,6-Oxaoctanedioic acid ($\mu = 1.0$)	3.055	3.676		
Oxoacetic acid	3.46			
2-Oxabutanedioic acid (oxaloacetic	2.56	4.27		
acid)	2.56	4.37		
2-Oxobutanoic acid	2.50			
5-Oxohexanoic acid (5-ketohexanoic	1.660			
acid) (18°C)	4.662			
3-Oxo-1,5-pentanedioic acid	3.10			
4-Oxopentanoic acid (levulinic acid)	4.59			
2-Oxopropanoic acid (pyruvic acid)	2.49			

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Oxytetracycline	3.10(+1)	7.26	9.11	
Papaverine	5.90(+1)			
Pentamethylenebis(thioacetic acid)	0.50(+1)			
(18°C)	3.485	4.413		
3,3-Pentamethylenepentanedioic	21.05			
acid	3.49	6.96		
1,5-Pentanediamine	10.05(+2)	10.916(+1)		
2,4-Pentanedione	8.24(enol);	10.510(+1)		
2,11 chancarone	8.95(keto)			
1-Pentanoic acid (valeric acid)	4.842			
2-Pentenoic acid	4.70			
3-Pentenoic acid	4.52			
4-Pentenoic acid	4.677			
Pentylarsonic acid	4.14	9.07		
N-Pentylveratramine	7.28(+1)	7.07		
Perhydrodiphenic acid (20°C)	4.96	6.68		
Perlolidine (18°C)	4.01	11.39		
Peroxyacetic acid	8.20	11.57		
1,7-Phenanthroline	4.30(+1)			
1,10-Phenanthroline	4.857(+1)			
6,7-Phenanthroline	4.857(+1)			
Phenazine	1.2(+1)			
Phenethylthioacetic acid	3.795			
Phenol	9.99			
Phenol-3-phosphoric acid	1.78	7.03	10.2	
Phenol-4-phosphoric acid	1.99	7.25	9.9	
Phenolphthalein	9.4			
3-Phenolsulfonic acid	7.1	9.05(-1)		
Phenolsulfonephthalein	7.9	7.05(1)		
Phenoxyacetic acid	3.171			
2-Phenoxybenzoic acid	3.53			
3-Phenoxybenzoic acid	3.95			
4-Phenoxybenzoic acid	4.52			
5-Phenoxy-1,2,3,4-tetrazole	3.49(+1)			
Phenylacetic acid	4.312			
L-3-Phenyl-α-alanine	2.16(+1)	9.31(0)		
3-Phenyl- α -alanine, methyl ester	7.05(+1)	7.01(0)		
Phenylalanylarginine ($\mu = 0.01$)	2.66(+1)	7.57(0)	12.40(-1)	
Phenylalanylglycine ($\mu = 0.01$)	3.10(+1)	7.71(0)	-2(1)	
7-Phenylazo-8-hydroxy-	0.10(11)	1(0)		
5-quinolinesulfonic acid	3.41(0)	7.850(-1)		



1,10-Phenanthroline

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK ₄
5-Phenylbarbituric acid	2.544(+1)			
2-Phenyl-2-benzylsuccinic acid	3.69	6.47		
1-Phenylbiguanide	2.13(+2)	10.76(+1)		
4-Phenylbutanoic acid	4.757			
Phenylbutazone	4.5(+1)			
2-Phenylenediamine	<2(+2)	4.47(+1)		
3-Phenylenediamine	2.65(+2)	4.88(+1)		
4-Phenylenediamine	3.29(+2)	6.08(+1)		
2-Phenylethylamine	9.83(+1)	. ,		
β-Phenylethylboronic acid	10.0			
DL-α-Phenylglycine	1.83(+1)	4.39(0)		
Phenylguanidine	10.77(+1)			
Phenylhydrazine	5.20(+1)			
2-Phenyl-3-hydroxypropanoic acid	3.53			
3-Phenyl-3-hydroxypropanoic acid	4.40			
Phenyliminodiacetic acid (20°C)	2.40	4.98		
Phenylmalonic acid	2.58	5.03		
Phenylmethanethiol	10.70			
2-Phenyl-2-phenethylsuccinic acid				
(20°C)	3.74	6.52		
2-Phenylphenol	9.55			
3-Phenylphenol	9.63			
4-Phenylphenol	9.55			
Phenylphosphinic acid (17°C)	2.1			
Phenylphosphonic acid	1.83	7.07		
O-Phenylphosphorylserine	2.13(+1)	8.79		
O-Phenylphosphorylserylglycine	3.18(+1)	6.95(0)		
O-Phenylphosphoryl-L-seryl-	\			
L-leucine	3.16(+1)	7.12(0)		
<i>N</i> -Phenylpiperazine ($\mu = 0.1$)	8.71(+1)			
2-Phenylpropanoic acid	4.38			
3-Phenylpropanoic acid (35°C)	4.664			
3-Phenyl-1-propylamine	10.39(+1)			
Phenylpropynoic acid (35°C)	2.269			
Phenylselenic acid	4.79			
Phenylselenoacetic acid ($\mu = 0.1$)	3.75			
β -Phenylserine ($\mu = 0.16$)	8.79(0)			
Phenylsuccinic acid (20°C)	3.78	5.55		
Phenylsulfenylacetic acid	2.66			
Phenylsulfonylacetic acid	2.44			
5-Phenyl-1,2,3,4-tetrazole	4.38(+1)			
1-Phenyl-1,2,3-triazole-4-carboxylic				
acid	2.88			
1-Phenyl-1,2,3-triazole-				
4,5-dicarboxylic acid	2.13	4.93		
Phosphoramidic acid	3.08	8.63		
O-Phosphorylethanolamine	5.838(+1)	10.638(0)		
O-Phosphorylserylglycine	3.13	5.41	8.01	

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
O-Phosphoryl-L-seryl-L-leucine	3.11	5.47	8.26	
Phosphoserine	2.08	5.65	9.74	
Phthalamide	3.79(0)			
Phthalazine	3.47(+1)			
o-Phthalic acid	2.950	5.408		
Phthalimide	9.90(0)			
Physostigmine	1.76(+1)	7.88(0)		
Picric acid (2,4,6-trinitrophenol)				
(18°C)	0.419			
Pilocarpine	1.3(+1)	6.85(0)		
Piperazine	5.333(+2)	9.781(+1)		
1,4-Piperazinebis(ethanesulfonic				
acid) (20°C)	6.80			
Piperazine-2-carboxylic acid	1.5	5.41	9.53	
Piperidine	11.123(+1)			
2-Piperidinecarboxylic acid	2.12(+1)	10.75(0)		
3-Piperidinecarboxylic acid	3.35(+1)	10.64(0)		
4-Piperidinecarboxylic acid	3.73(+1)	10.72(0)		
1-(2-Piperidinyl)-2-propanone (15°C)	9.45			
Piperine (15°C)	1.98(+1)			
Proline	1.952(+1)	10.640(0)		
1,2-Propanediamine	6.607(+2)	9.720(+1)		
1,3-Propanediamine	8.49(+2)	10.47(+1)		
1-Propanethiol	10.86			
1,2,3-Propanetriamine	3.72(+3)	7.95(+2)	9.59(+1)	
1,2,3-Propanetricarboxylic acid	3.67	4.87	6.38	
Propanoic acid	4.874			
Propenoic acid	4.247			
N-Propionylglycine	3.718(0)			
2-Propoxybenzoic acid (20°C)	4.24			
3-Propoxybenzoic acid (20°C)	4.20			
4-Propoxybenzoic acid (20°C)	4.78			
N-Propylalanine	2.21(+1)	10.19(0)		
Propylamine	10.568(+1)			
Propylarsonic acid (18°C)	4.21	9.09		
Propylenimine	8.18(+1)			
<i>N</i> -Propylglycine ($\mu = 0.1$)	2.38(+1)	10.03(0)		
L-Propylglycine	3.19(+1)	8.97(0)		
Propylmalonic acid	2.97	5.84		
Propylphosphinic acid	3.46			

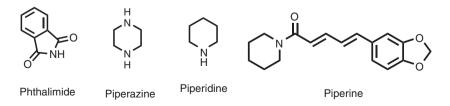


TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK_4
Propylphosphonic acid	2.49	8.18		
2-Propylpyridine	6.30(+1)			
<i>N</i> -Propylveratramine	7.20(+1)			
2-Propynoic acid	1.887			
Pseudoecgonine	9.70			
Pseudoisocyanine ($\mu = 0.2$)	4.59(+2)			
Pseudotropine	9.86(+1)			
Pteroylglutamic acid	8.26			
Purine	2.52(+1)	8.92(0)		
Pyrazine	0.6(+1)			
Pyrazinecarboxamide	0.5(+1)			
Pyrazole	2.61(+1)			
Pyridazine	2.33(+1)			
Pyridine	5.17(+1)			
Pyridine-d ₅	5.83(+1)			
2-Pyridinealdoxime	3.56(+1)	10.17(0)		
3-Pyridinealdoxime	4.07(+1)	10.39(0)		
4-Pyridinealdoxime	4.73(+1)	10.03(0)		
2-Pyridinecarbaldehyde	3.84(+1)			
3-Pyridinecarbaldehyde	3.80(+1)			
4-Pyridinecarbaldehyde	4.74(+1)			
3-Pyridinecarbamide (nicotinamide)	3.33(+1)			
3-Pyridinecarbonitrile	1.35(+1)			
Pyridine-2-carboxylic acid				
(picolinic acid)	1.01(+1)	5.29(0)		
Pyridine-3-carboxylic acid				
(nicotinic acid)	2.07(+1)	4.75(0)		
Pyridine-4-carboxylic acid				
(isonicotinic acid)	1.84(+1)	4.86(0)		
Pyridine-2,3-dicarboxylic acid	2.36(+1)	7.08(0)		
Pyridine-2,4-dicarboxylic acid	2.23(+1)	7.02(0)		
Pyridine-2,6-dicarboxylic acid	2.16(+1)	6.92(0)		
Pyridine-1-oxide	0.688(+1)			
Pyridoxal	4.20(+1)	8.66(ring		
		OH)		
Pyridoxal-5-phosphate ($\mu = 0.15$)	< 2.5	4.14	6.20	8.69
Pyridoxamine ($\mu = 0.1$)	3.37(+2)	8.01(+1)	10.13(ring OH)	
Pyridoxamine-5-phosphate				
$(\mu = 0.15; pK_5 = 10.92)$	2.5	3.69	5.76	8.61
Pyridoxine (vitamin B ₆) (18 °C)	5.00(+1)	8.96(ring		
0, (- 0)		OH)		











Purine

Pyrazine

Pyrazole

Pyridazine

Pyridine

8.54 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK ₃	pK_4
3-(2'-Pyridyl)alanine	1.37(+2)	4.02(+1)	9.22(0)	
3-(3'-Pyridyl)alanine	1.77(+2)	4.64(+1)	9.10(0)	
2-(2'-Pyridyl)benzimidazole				
$(\mu = 0.16)$	5.58(+1)			
2-(2'-Pyridyl)imidazole ($\mu = 0.005$)	8.98(+1)			
4-(2'-Pyridyl)imidazole ($\mu = 0.1$)	5.49(+1)			
Pyrimidine	1.30(+1)			
2,4(1 <i>H</i> ,3 <i>H</i>)-Pyrimidinedione				
(uracil)	0.6(+1)	9.46(0)		
2,4,5,6(1H,3H)-Pyrimidinetetrone-				
5-oxime	4.57(0)			
Pyrocatecholsulfonephthalein	7.82	9.76	11.73	
Pyroxilidine	11.11(+1)			
Pyrrole-1-carboxylic acid	4.45			
Pyrrole-2-carboxylic acid	4.45			
Pyrrole-3-carboxylic acid	4.453			
Pyrrolidine	11.305(+1)			
Pyrrolidine-2-carboxylic acid				
(proline)	1.952(+1)	10.640(0)		
2-[2-(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	3.60(+2)	9.39(+1)		
3-[2-(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	4.28(+2)	9.28(+1)		
4-[2(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	4.65(+2)	9.27(+1)		
2-(1-Pyrrolidinylmethyl)pyridine	2.54(+1)	8.56(+1)		
3-(1-Pyrrolidinylmethyl)pyridine	3.14(+2)	8.36(+1)		
4-(1-Pyrrolidinylmethyl)pyridine	3.38(+2)	8.16(+1)		
3-Pyrroline	-0.27(+1)			
Ovinidina	4.0(+1)	9.54(0)		
Quinidine	4.0(+1)	8.54(0)		
Quinine	4.11(+1)	8.52(0)		
Quinoline	4.80(+1)			
Quinoxaline	0.72(+1)			
D-Raffinose	12.74			
Riboflavin (vitamin B_2) ($\mu = 0.01$)	ca -0.2	9.69		
α -D-Ribofuranose	12.11			
D-Ribose-5'-phosphonic acid		6.70(-1)	13.05(-2)	

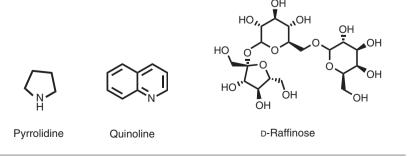


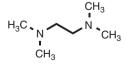
TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Substance	pK ₁	pK ₂	pK ₃	pK_4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	D-Saccharic acid	5.00(0)			
Sarcosine Sarcosine amide Sarcosine amide Sarcosine amide Sarcosine dimethylamide Sarcosine dimethylamide Sarcosylgycine ($\mu=0.16$) Sarcosylgycine ($\mu=0.16$) 3.15(+1) 8.56(0) Sarcosylgycine ($\mu=0.16$) 3.15(+1) 8.67(0) Sarcosylserine 3.15(+1) 8.63(0) 3.292(+1) 9.15(0) Sarcosylserine 3.17(+1) 8.63(0) 3.292(+1) 9.15(0) Sarcosylserine 3.17(+1) 8.63(0) 3.292(+1) 9.208(0) Serine, methyl ester ($\mu=0.1$) 3.53(+1) 1.2-Serine 2.186(+1) 9.208(0) Serine, methyl ester ($\mu=0.1$) 7.03(+1) Serylglycine ($\mu=0.15$) 2.10(+1) 7.33(0) 3.08(+1) 7.45(0) Solanine 7.34(+1) 10.5 Solanine 7.34(+1) 10.5 Solanine 7.34(+1) 10.5 Solanine 7.34(+1) 10.5 Solanine 7.34(+1) 11.76(0) Spinaceamine ($\mu=0.1$) 4.895(+2) 8.90(+1) Spinacine 4.49(+1) 11.76(0) Spinacine ($\mu=0.1$) 4.895(+2) 8.90(+1) Spinacine 1.649(+2) 4.936(+1) 8.663(0) 10.5 Succinamic acid (succinic acid monoamide) 4.39(0) Succinamic acid (succinic acid monoamide) 4.39(0) Succinamic acid (succinic acid 3.54 4.5ulfamilonphenyl)alanine 3.5ulfamylbenzoic acid 3.54 4.Sulfamylphenylphosphoric acid 3.54 4.Sulfamylphenylphosphoric acid 3.54 4.Sulfamylphenylphosphoric acid 3.54 4.Sulfamylphenylone 10.39 9.07 4.5ulfophenol 0.58 8.70 1.99 5.Sulfosalicylic acid 7.62	Saccharin (o-benzoic sulfimide)	2.32			
Sarcosine dimethylamide Sarcosine methylamide Sarcosine methylamide Sarcosine methylamide Sarcosylglycine $(\mu=0.16)$ Sarcosylglycine $(\mu=0.16)$ Sarcosylglycine $(\mu=0.16)$ Sarcosylglycine $(\mu=0.16)$ Sarcosylglycine $(\mu=0.1)$ Sarcosylgrine Sarcosylserine Sarcosylserine $(\mu=0.1)$ Sarcosylserine $($		2.12(+1)	10.20(0)		
Sarcosine methylamide Sarcosylglycine ($\mu = 0.16$) 3.15(+1) 8.56(0) 3.15(+1) 8.67(0) Sarcosylgucine 3.15(+1) 8.67(0) Sarcosylserosine 3.17(+1) 9.15(0) Sarcosylserine 3.17(+1) 8.63(0) Sarcosylserine 3.17(+1) 8.63(0) Sarcosylserine 3.17(+1) 8.63(0) Sarcosylserine 3.17(+1) 8.63(0) Selenosemicarbazide ($\mu = 0.1$) $0.8(+1)$ Semicarbazide ($\mu = 0.1$) $0.8(+1)$ Serine, methyl ester ($\mu = 0.1$) $0.8(+1)$ Serine, methyl ester ($\mu = 0.1$) $0.8(+1)$ 0	Sarcosine amide	8.35(+1)	. , ,		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Sarcosine dimethylamide	` ′			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Sarcosine methylamide	8.28(+1)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		3.15(+1)	8.56(0)		
Sarcosylserine 3-Selenosemicarbazide $(\mu = 0.1)$	Sarcosylleucine	3.15(+1)	8.67(0)		
3-Selenosemicarbazide ($μ = 0.1$) Semicarbazide ($μ = 0.1$) Serine Serine, methyl ester ($μ = 0.1$) 3.53(+1) 2.186(+1) 7.03(+1) 3.53(+1) 2.186(+1) 7.33(0) 3.08(+1) 7.34(+1) 3.59r1-L-leucine 3.08(+1) 7.34(+1) 3.59rateine 3.08(+1) 7.34(+1) 3.59rateine 3.08(+1) 7.45(0) 7.34(+1) 3.60 11.55 3.60 11.55 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.60	Sarcosylsarcosine	2.92(+1)	9.15(0)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Sarcosylserine	3.17(+1)	8.63(0)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3-Selenosemicarbazide ($\mu = 0.1$)	0.8(+1)	` '		
Serine, methyl ester ($\mu = 0.1$) Serylglycine ($\mu = 0.15$) L-Seryl-L-leucine Solanine D-Sorbitol (17.5 °C) Sparteine Spinaceamine ($\mu = 0.1$) Spinaceamine ($\mu = 0.1$) Spinaceamine ($\mu = 0.1$) Spinaceine L-Strychnine (15 °C) Succinamic acid (succinic acid monoamide) Succinic acid D-Succinimide S-Sulfamylbenzoic acid 4-Sulfamylbenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 4-Sulfophenol 2-Sulfophenol 2-Sulfophenol 2-Sulfopropanoic acid Sylvic acid 10.0 7.03(+1) 2.10(+1) 7.33(0) 7.45(0) 7.45(0) 7.45(0) 7.45(0) 7.45(0) 7.45(0) 7.45(0) 7.45(0) 8.663(0	Semicarbazide ($\mu = 0.1$)	3.53(+1)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Serine	2.186(+1)	9.208(0)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Serine, methyl ester ($\mu = 0.1$)	7.03(+1)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Serylglycine ($\mu = 0.15$)	2.10(+1)	7.33(0)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		3.08(+1)	7.45(0)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Solanine	7.34(+1)	` '		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	o-Sorbitol (17.5°C)	13.60			
Spinaceamine ($\mu = 0.1$) 4.895(+2) 8.90(+1) Spinacine 1.649(+2) 4.936(+1) 8.663(0) L-Strychnine (15 °C) 2.50 8.20 Succinamic acid (succinic acid monoamide) 4.39(0) 4.207 5.635 Succinimide 9.623 5.635 9.623 3-C4'-Sulfaminophenyl)alanine 1.99(+1) 8.64(0) 10.26(-1) 3-Sulfamylbenzoic acid 3.54 3.47 4.26 3.8 4-Sulfamylphenylphosphoric acid 10.43(+1) 4.0 3.78 3.72 3-Sulfobenzoic acid 3.72 3.72 3.72 3.72 3.72 3.72 3-Sulfophenol 0.58 8.70 2.5ulfophenol 2.49 12.00 5.01 5.01 5.01 5.00 <td>L-(-)-Sorbose (18°C)</td> <td>11.55</td> <td></td> <td></td> <td></td>	L-(-)-Sorbose (18°C)	11.55			
Spinacine	Sparteine	4.49(+1)	11.76(0)		
Spinacine	Spinaceamine ($\mu = 0.1$)	4.895(+2)	8.90(+1)		
Succinamic acid (succinic acid monoamide) Succinic acid L-Succinimide S-Sulfamilophenyl)alanine S-Sulfamylbenzoic acid S-Sulfamylphenylphosphoric acid S-Sulfobenzoic acid S-Sulfobenzoic acid S-Sulfophenol S-		1.649(+2)		8.663(0)	
monoamide) Succinic acid OL-Succinimide 3-Sulfaminophenyl)alanine 3-Sulfamylbenzoic acid 4-Sulfamylphenylphosphoric acid 4-Sulfamilamide Sulfanilamide Sulfoacetic acid 3-Sulfobenzoic acid 4-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 4-Sulfophenol 4-Sulfophenol 5-Sulfophenol 6-Sulfophenol 7-Sulfophenol	L-Strychnine (15°C)	2.50	8.20		
Succinic acid OL-Succinimide 3-(4'-Sulfaminophenyl)alanine 3-Sulfamylbenzoic acid 4-Sulfamylbenzoic acid 4-Sulfamylphenylphosphoric acid 3.54 4-Sulfamylphenylphosphoric acid 5-Sulfophenol 2-Sulfophenol 2-Sulfophenol 3-Sulfophenol 2-Sulfophenol 2-Sulfophenol 3-Sulfophenol 2-Sulfophenol 3-Sulfophenol 3-Sulfophe	Succinamic acid (succinic acid				
Solution	monoamide)	4.39(0)			
3-(4'-Sulfaminophenyl)alanine 3-Sulfamylbenzoic acid 4-Sulfamylbenzoic acid 4-Sulfamylphenylphosphoric acid 5-Sulfoacetic acid 3.54 3.47 1.42 10.43(+1) 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 4-Sulfophenol 5-Sulfophenol 2-Sulfopropanoic acid 5-Sulfosalicylic acid 8-Sulfosalicylic acid 7.62	Succinic acid	4.207	5.635		
3-Sulfamylbenzoic acid 4-Sulfamylbenzoic acid 4-Sulfamylphosphoric acid 4-Sulfamylphosphoric acid 5-Sulfoacetic acid 3.54 3.47 1.42 10.43(+1) 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 0.39 4-Sulfophenol 0.58 8.70 2-Sulfopropanoic acid 5-Sulfosalicylic acid 3.72 3-Sulfophenol 0.58 8.70 2-Sulfosalicylic acid 5-Sulfosalicylic acid 7.62	DL-Succinimide	9.623			
4-Sulfamylbenzoic acid 4-Sulfamylphenylphosphoric acid 5-Sulfoacetic acid 3.47 1.42 10.43(+1) 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 4-Sulfophenol 4-Sulfophenol 5-Sulfophenol 2-Sulfopropanoic acid 5-Sulfosalicylic acid 8-Sylvic acid 3.72 3.72 3.72 3.72 3.72 3.72 3.72 3.72	3-(4'-Sulfaminophenyl)alanine	1.99(+1)	8.64(0)	10.26(-1)	
4-Sulfamylphenylphosphoric acid Sulfanilamide Sulfoacetic acid 3-Sulfobenzoic acid 4-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 4-Sulfophenol 4-Sulfophenol 5-Sulfophenol 2-Sulfophenol 2-Sulfophenol 2-Sulfophenol 3-Sulfophenol 4-Sulfophenol 5-Sulfophenol 7-Sulfosalicylic acid 8-Sylvic acid 7-62	3-Sulfamylbenzoic acid	3.54			
4-Sulfamylphenylphosphoric acid Sulfanilamide Sulfoacetic acid 3-Sulfobenzoic acid 4-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 4-Sulfophenol 4-Sulfophenol 5-Sulfophenol 2-Sulfophenol 2-Sulfophenol 2-Sulfophenol 3-Sulfophenol 4-Sulfophenol 5-Sulfophenol 7-Sulfosalicylic acid 8-Sylvic acid 7-62	4-Sulfamylbenzoic acid	3.47			
Sulfoacetic acid 3-Sulfobenzoic acid 4-Sulfobenzoic acid 3-Sulfophenol 3-Sulfophenol 4-Sulfophenol 4-Sulfophenol 5-Sulfophenol 5-Sulfosalicylic acid 6-Sylvic acid 7.62		1.42	6.38	10.0	
3-Sulfobenzoic acid 4-Sulfobenzoic acid 3-Sulfobenzoic acid 3-Sulfophenol 0.39 4-Sulfophenol 0.58 8.70 2-Sulfopropanoic acid 1.99 5-Sulfosalicylic acid 2.49 12.00 Sylvic acid 7.62	Sulfanilamide	10.43(+1)			
4-Sulfobenzoic acid 3-Sulfophenol 0.39 9.07 4-Sulfophenol 0.58 8.70 2-Sulfopropanoic acid 5-Sulfosalicylic acid 2.49 7.62	Sulfoacetic acid		4.0		
3-Sulfophenol 0.39 9.07 4-Sulfophenol 0.58 8.70 2-Sulfopropanoic acid 1.99 5-Sulfosalicylic acid 2.49 12.00 Sylvic acid 7.62	3-Sulfobenzoic acid		3.78		
4-Sulfophenol 0.58 8.70 2-Sulfopropanoic acid 1.99 5-Sulfosalicylic acid 2.49 12.00 Sylvic acid 7.62	4-Sulfobenzoic acid		3.72		
2-Sulfopropanoic acid 1.99 5-Sulfosalicylic acid 2.49 12.00 Sylvic acid 7.62	3-Sulfophenol	0.39	9.07		
2-Sulfopropanoic acid 1.99 5-Sulfosalicylic acid 2.49 12.00 Sylvic acid 7.62	1-Sulfophenol	0.58	8.70		
Sylvic acid 7.62	1	1.99			
Sylvic acid 7.62		2.49	12.00		
		7.62			
0-1artaric acid 3.000 4.000			1 366		
meso-Tartaric acid 3.22 4.81					

8.56 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK_2	pK_3	pK_4
Tetracycline ($\mu = 0.005$)	3.30(+1)	7.68	9.69	
Tetradehydroyohimbine	10.59(+1)			
Tetraethylenepentamine				
$[\mu = 0.1; pK_5 = 9.67(+1)]$	2.98(+5)	4.72(+4)	8.08(+3)	9.10(+2)
1,4,5,6-Tetrahydro-				
1,2-dimethylpyridine	11.38(+1)			
1,4,5,6-Tetrahydro-2-methylpyridine	9.53(+1)			
cis-Tetrahydronaphthalene-				
2,3-dicarboxylic acid (20°C)	3.98	6.47		
trans-Tetrahydronaphthalene-				
2,3-dicarboxylic acid (20°C)	4.00	5.70		
5,6,7,8-Tetrahydro-1-naphthol	10.28			
5,6,7,8-Tetrahydro-2-naphthol	10.48			
Tetrahydroserpentine	10.55(+1)			
2,3,5,6-Tetramethylbenzoic acid	3.415			
Tetramethylenebis(thioacetic acid)				
(18°C)	3.463	4.423		
Tetramethylenediamine	9.22(+2)	10.75(+1)		
N,N,N',N'-				
Tetramethylethylenediamine	2.20(+2)	6.35(+1)		
2,3,5,6-Tetramethyl-				
4-methylaminopyridine	0.07(+1)			
2,2,6,6-Tetramethylpiperidine				
$(\mu = 0.5)$	1.24(+1)			
2,3,5,6-Tetramethylpyridine (20°C)	7.90(+1)			
Tetramethylsuccinic acid	3.50	7.28		
1,2,3,4-Tetrazole	4.90			
Thebaine	7.95(+1)			
2-Thenoyltrifluoroacetone	5.70(0)			
Theobromine	0.68(+1)	7.89		
Theophylline	< 1(+1)	8.80		
Thiazoline	2.53(+1)			
Thioacetic acid	3.33			
o-Thiocresol	6.64			
m-Thiocresol	6.58			
p-Thiocresol	6.52			
Thiocyanatoacetic acid	2.58			
2,2'-Thiodiacetic acid	3.32	4.29		
4,4'-Thiodibutanoic acid (18°C)	4.351	5.275		



N NH N N



N,N,N,N-Tetramethylethylenediamine

1,2,3,4-Tetrazole

Thiazoline

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK_2	pK ₃	pK_4
3,3'-Thiodipropanoic acid (18°C)	4.085	5.075		
3-Thio-S-methylcarbazide ($\mu = 0.1$)	7.563(+1)			
1-Thionylcarboxylic acid	3.53			
2-Thionylcarboxylic acid	4.10			
2-Thiophenecarboxylic acid (30°C)	3.529			
3-Thiophenecarboxylic acid				
(3-thenoic acid)	4.10			
Thiophenol	6.50			
3-Thiosemicarbazide ($\mu = 0.1$)	1.5(+1)			
3-Thiosemicarbazide-1,1-diacetic				
acid (30°C)	2.94	4.07		
Thiourea	2.03(+1)			
Thorin	3.7	8.3	11.8	
Thymidine	9.79	12.85		
p-Toluenesulfinic acid	1.7			
Toluhydroquinone	10.03	11.62		
o-Toluidine	4.45(+1)			
<i>m</i> -Toluidine	4.71(+1)			
<i>p</i> -Toluidine	5.08(+1)			
o-Tolylacetic acid (18°C)	4.36			
p-Tolylacetic acid (18°C)	4.36			
o-Tolylarsonic acid	3.82	8.85		
m-Tolylarsonic acid	3.82	8.60		
p-Tolylarsonic acid	3.70	8.68		
o-Tolylphosphonic acid	2.10	7.68		
m-Tolylphosphonic acid	1.88	7.44		
p-Tolylphosphonic acid	1.84	7.33		
3-Tolylselenic acid	4.80			
4-Tolylselenic acid	4.88			
Triacetylmethane	5.81			
Triallylamine	8.31(+1)			
1,3,5-Triazine-2,4,6-triol	7.20	11.10		
1 <i>H</i> -1,2,3-Triazole		9.26		
1 <i>H</i> 1,2,4-Triazole	2.386(+1)	9.972		
1,2,3-Triazole-4-carboxylic acid	3.22	8.73		
1,2,3-Triazole-4,5-dicarboxylic acid	1.86	5.90	9.30	
1,2,4-Triazolidine-3,5-dione (urazole)	5.80			
Tribromoacetic acid	-0.147			
2,4,6-Tribromobenzoic acid	1.41			
Trichloroacetic acid	0.52			
Trichloroacrylic acid	1.15			

Thymidine

$$H_2N$$

o-Toluidine

8.58 SECTION 8

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3,3,3-Trichlorolactic acid	2.34			
Trichloromethylphosphonic acid	1.63	4.81		
2,4,5-Trichlorophenol	7.37			
3,4,5-Trichlorophenol	7.839			
Tricine (20°C)	8.15			
Triethanolamine	7.76(+1)			
Triethylamine	10.72(+1)			
Triethylenediamine	4.18(+2)	8.19(+1)		
Triethylenetetramine (20°C)	3.32(+4)	6.67(+3)	9.20(+2)	9.92(+1)
Triethylsuccinic acid	2.74	,	,	
Trifluoroacetic acid	0.50			
Trifluoroacrylic acid	1.79			
4,4,4-Trifluoro-2-aminobutanoic acid	1.600(+1)	8.169(0)		
4,4,4-Trifluoro-3-aminobutanoic acid	2.756(+1)	5.822(0)		
4,4,4-Trifluorobutanoic acid	4.16	210=2(0)		
α, α, α -Trifluoro- <i>m</i> -cresol	8.950			
4,4,4-Trifluorocrotonic acid	3.15			
5,5,5-Trifluoroleucine	2.045(+1)	8.942(0)		
3-(Trifluoromethyl)aniline	3.5(+1)	0.5 .2(0)		
4-(Trifluoromethyl)aniline	2.6(+1)			
3-Trifluoromethylphenol	8.950			
5-Trifluoromethyl-1,2,3,4-tetrazole	1.70			
6,6,6-Trifluoronorleucine	2.164(+1)	9.463(0)		
5,5,5-Trifluoronorvaline	2.042(+1)	8.916(0)		
5,5,5-Trifluoropentanoic acid	4.50	0.510(0)		
3,3,3-Trifluoropropanoic acid	3.06			
4,4,4-Trifluorothreonine	1.554(+1)	7.822(0)		
4,4,4-Trifluorovaline	1.537(+1)	8.098(0)		
1,2,3-Trihydroxybenzene	1.007(+1)	0.050(0)		
(pyrogallol)	9.03(0)	11.63(-1)		
1,3,5-Trihydroxybenzene	8.45(0)	8.88(-1)		
(phloroglucinol)	0.15(0)	0.00(1)		
2,4,6-Trihydroxybenzoic acid	1.68(0)			
3,4,5-Trihydroxybenzoic acid	4.19(0)	8.85(-1)		
3,4,5-Trihydroxycyclohex-1-ene-	,(0)	0.05(1)		
1-carboxylic acid				
[D-(-)-shikimic acid]	4.15			
2,4,6-Tri(hydroxymethyl)phenol	9.56			
Triisobutylamine	10.42(+1)			
Trimethylamine	9.80(+1)			
3-(Trimethylamino)phenol	8.06			
4-(Trimethylamino)phenol	8.35			
2,4,6-Trimethylaniline	4.38(+1)			
2,4,6-Trimethylbenzoic acid	3.448			
Trimethylenebis(thioacetic acid) (18°C)	3.435	5.383		
2,3,4-Trimethylphenol	10.59			
2,4,5-Trimethylphenol	10.57			
2,4,6-Trimethylphenol	10.88			
3,4,5-Trimethylphenol	10.25			
2,3,6-Trimethylpyridine ($\mu = 0.5$)	7.60(+1)			
				<u></u>

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK ₂	pK ₃	pK_4
2,4,6-Trimethylpyridine	7.43(+1)			
2,4,6-Trimethylpyridine-1-oxide	1.990(+1)			
3-(Trimethylsilyl)benzoic acid	4.089			
4-(Trimethylsilyl)benzoic acid	4.192			
2,4,5-Trimethylthiazole ($\mu = 0.1$)	4.55			
2,4,6-Trinitroaniline (picramide)	-10.23(+1)			
2,4,6-Trinitrobenzene acid	0.654			
2,2,2-Trinitroethanol	2.36			
Trinitromethane (20°C)	0.17			
Triphenylacetic acid	3.96			
Tripropylamine	10.66(+1)			
Tris(2-hydroxyethyl)amine	7.762(+1)			
Tris(hydroxymethyl)aminomethane	, , ,			
(TRIS)	8.08(+1)			
2-[Tris(hydroxymethyl)methyl	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \			
amino]-1-ethanesulfonic acid				
(TES)	7.50			
3-[Tris(hydroxymethyl)methyl				
amino]-1-propanesulfonic acid				
(TAPS) (20°C)	8.4			
<i>N</i> -[Tris(hydroxymethyl)methyl]-				
glycine (tricine)	2.023(+1)	8.135		
Tris(trimethylsilyl)amine	4.70(+1)			
Trithiocarbonic acid (20°C)	2.64			
Tropacocaine (15°C)	9.88(+1)			
3-Tropanol (tropine)	10.33(+1)			
Trypsin ($\mu = 0.1$)	6.25			
L-Tryptophan	2.38(+1)	9.39(0)		
DL-Tyrosine	2.18(+1)	9.21(0)	10.47(OH)	
Tyrosine amide	7.48	9.89	` ′	

Tris(hydroxymethyl)aminomethane

2-[Tris(hydroxymethyl)methylamino]-1-ethanesulfonic acid

3-[Tris(hydroxymethyl)methylamino]-1-propanesulfonic acid

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TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK_1	pK_2	pK ₃	pK_4
Tyrosine, ethyl ester Tyrosylarginine ($\mu = 0.01$) Tyrosyltyrosine	7.33 2.65(+1) 3.52(+1)	9.80 7.39(0) 7.68(0)	9.36(-1) 9.80(-1)	11.62(-2) 10.26(-2)
α -Ureidobutanoic acid γ -Ureidobutanoic acid β -Ureidopropanoic acid Uric acid Uridine Uridine-5'-diphosphoric acid Uridine-5'-phosphoric acid (5'-uridylic acid) Uridine-5'-triphosphoric acid	3.886(0) 4.683(0) 4.487(0) 5.40 9.30 7.16 6.63 7.58	5.53		
DL-Valine L-Valine Valine amide ($\mu=0.2$) L-Valine, methyl ester L-Valylglycine	2.286(+1) 2.296(+1) 8.00 7.49(+1) 3.23(+1)	9.719(0) 9.79(0) 8.00(0)		
Vetramine Veratrine Vinylmethylamine 2-Vinylpyridine 4-Vinylpyridine Vitamin B ₁₂	7.49(+1) 8.85(+1) 9.69(+1) 4.98(+1) 5.62(+1) 7.64(+1)			
Xanthine (40 °C) Xanthosine Xylenol Orange [pK ₅ = 10.46(-4);	0.68(+1) < 2.5(+1)	5.67(0)	12.00(-1)	
$pK_6 = 12.28(-5)$] D-(+)-Xylose	12.15(0)	2.58(-1)	3.23(-2)	6.37(-3)
Zincon		4	7.85	15

Table 8.2 records the acidities of inorganic compounds expressed as their pK_A values (see page 8.2 for a discussion of pK_A). When more than one ionizable proton is present, pK_1 , pK_2 , etc. values are given. Cations formed from the indicated compound by protonation are indicated by "(+1)" or "(+2)" for a dication.

Temperature values different from 25 °C are given in parentheses as are other relevant variations. For example, the dissociation constant for acetic acid- d_1 is reported in D_2O .

TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °C

The protonation states of cations are designated by values (+1), (+2), etc. that follow pK_A values.

Substance	Formula	pK_1	pK_2	pK ₃	pK_4
Aluminic acid (alumina)	H ₃ AlO ₃	11.2			
Amidophosphoric acid	H ₂ NPO(OH) ₂	3.3	8.28	0.70	
Aminodisulfonic acid	HN(SO ₃ H) ₂	0.24		8.50	
Ammonium ion	NH ₄ ⁺	9.24	6.77	11.50	
Arsenic acid	H ₃ AsO ₄	2.25	6.77	11.53	
Arsenous acid	HAsO ₂ or HAs(OH) ₄	9.23	12.74		
Boric acid, ortho- Boric acid, etra-	H_3BO_3 $H_2B_4O_7$	9.236 4	12.74 9		
Carbonic acid	$ \begin{array}{c} H_2B_4O_7\\ CO_2 + H_2O \end{array} $	6.35	10.53		
Carbonic acid	(without including	0.55	10.55		
	dehydration constant)	3.76	10.329		
	$CO_2 + D_2O$ (solvent)	6.77	11.076		
Chloric acid	HClO ₃	-1.58	11.070		
Chlorous acid	HClO ₂	2.021			
Chlorosulfonic acid	HOSO ₂ C1	-10.43			
Chromic acid	H ₂ CrO ₄	-0.98	6.50		
Cyanic acid	HOCN	3.47	0.00		
Deuterium oxide	D ₂ O (solvent)	14.87			
Diamidophosphoric acid	$(H_2N)_2PO_2H$	4.83			
Dithionic acid	H ₂ S ₂ O ₆	-3.4	-0.2		
Dithionous acid	H ₂ S ₂ O ₄	0.35	2.45		
Ferricyanic acid	H ₃ Fe(CN) ₆	< 1			
Ferrocyanic acid	$H_2(Fe(CN)_6)^{2-}$			2.57	4.35
Fluorophosphoric acid	FPO(OH) ₂		4.79		
Hexapolyphosphoric acid	$H_8P_6O_{19}$	ca 2.1	2.19	5.98	8.13
Hydrazinium(2+) ion	+H ₃ NNH ₃ +	-0.88	7.956		
(20°C)		(+2)	(+1)		
Hydrazinosulfuric acid	H ₂ NNHSO ₃ H	3.85			
Hydrazoic acid	HN ₃	4.64			
Hydrocyanic acid	HCN	9.21			
Hydrogen bromide	HBr	-20.68			
Hydrogen chloride	HCl	-6.1			
Hydrogen fluoride	HF	3.17			
Hydrogen iodide	HI	-9.5			
Hydrogen peroxide Hydrogen polysulfide	H_2O_2	11.58			
(20°C)	H ₂ S ₄	3.8	6.3		
Hydrogen selenide	H ₂ Se	3.89	11.0		
Hydrogen sulfide	H ₂ Se	6.96	12.90		
Hydrogen telluride (20°C)	H ₂ Te	2.64	11–12		
Hydroperoxy radical	$HO_2=H^++O_2^-$	4.45	11 12		
Hydroxide radical	OH:	11.9			
Hydroxylamine- <i>N</i> , <i>N</i> -di		11.7			
sulfonic acid	HON(SO ₃ H) ₂			11.85	
Hydroxylamine- <i>N</i> -sulfonic	- 10 3 -72				
acid	HONH—OSO ₂ H		ca 12.5		
Hydroxylammonium ion	HONH ₃ ⁻	5.98			

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TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °C (continued)

Substance	Formula	pK_1	pK_2	pK ₃	pK ₄
Hypobromous acid	HBrO	8.597			
Hypochlorous acid	HClO	7.54			
Hypoiodous acid	HIO	10.64			
Hyponitrous acid	HON=NOH	7.05	11.54		
Hypophosphoric acid					
(20°C)	$H_4P_2O_6$	2	2.19		
Hypophosphorus acid	HPH,O,	1.23			
Hyposulfurous acid	$H_2S_2O_4$	0.35	2.45		
Imidodiphosphoric acid	(HO) ₂ PO—NH—				
1 1	PO(OH),	ca 2	2.85	7.08	9.72
Iodic acid (30°C)	HIO ₃	0.815			
Nitramide	O ₂ NNH ₂	6.48			
Nitric acid	HNO ₃	1.38			
Nitrous acid	HNO ₂	3.14			
Osmic acid	H ₂ OsO ₅ (mainly OsO ₄)	12.0	14.5		
Perchloric acid	HCIO ₄ (completely				
	dissociated up to				
	10M)				
Periodic acid, para-	H ₅ IO ₆	1.55	8.27		
Permanganic acid	HMnO ₄	-2.25			
Peroxide radical	HO ₅	4.90			
Peroxoboric acid	$H_3BO_3 + H_2O_2 =$				
	$(H_2BO_3 \cdot H_2O_2)^- + H^+$	7.91			
Peroxochromic acid	H ₂ CrO ₅	4.30			
Peroxomonosulfuric acid	H ₂ SO ₅	1.0	9.3		
Perxenic acid	H ₄ XeO ₆	ca 2	ca 6	ca 10	
Phosphoric acid, ortho-	H ₃ PO ₄	2.148	7.198	12.38	
Deuterated	D ₃ PO ₃	2.420	7.201		
Phosphoric acid, di-	$H_4P_2O_7$	0.91	2.10	6.70	9.38
Phosphorous acid (20°C)	H ₂ PHO ₃	1.20	6.70		
Selenic acid	H ₂ SeO ₄	-3	1.74		
Selenous acid	H ₂ SeO ₃	2.27	7.78		
Silicic acid	H ₂ SiO ₃	9.77	11.80		
Sulfamic acid	HOSO ₂ NH ₂	0.988			
Sulfuric acid	H ₂ SO ₄	ca - 3	1.987		
Sulfurous acid	$SO_2 + H_2O$ (includes				
	dehydration constant)	1.89	7.20		
Telluric acid	H ₆ TeO ₆	7.70	10.99		
Tellurous acid	H ₂ TeO ₃	2.46	7.7		
Tetraperoxochromic acid					
(30°C)	H ₃ CrO ₈	7.16			
Tetrapolyphosphoric acid					
$(pK_5 = 6.63; pK_6 = 8.34)$	$H_6P_4O_{13}$			1.3	2.23
Thiocyanic acid	HSCN	0.95			
Thiosulfuric acid	$H_2S_2O_3$	0.60	1.5–1.7		
Trimetaphosphoric acid	$H_3P_3O_4$			2.0	
Tripolyphosphoric acid	$H_5P_3O_{10}$	-0.51	1.20	2.30	6.61
$(\mu > 1)* (pK_5 = 9.26)$					
Trithiocarbonic acid	11.00	2.66	0.46		
(20°C)	H ₂ CS ₃	2.68	8.18		

TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °C (*continued*)

Substance	Formula	pK ₁	pK_2	pK ₃	pK ₄
Tungstic acid (20°C) Vanadic acid Water Xenon trioxide	$\begin{aligned} & & & H_2WO_4 \\ & & & H_3VO_4 \\ & & & H_2O \\ & & & XeO_3 \ (aqueous) = \\ & & & & HXeO_4^- + H^+ \end{aligned}$	ca 3.5 3.78 14.003	ca 4.6 7.8	13.0	

^{*} Ionic strength.

 TABLE 8.3
 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures

Abbreviations Used in the Table

(+1), monoprotonated cation (0), neutral molecule

(-1), monoanion (-2), dianion

 $pK_{\text{auto}},$ negative logarithm (base 10) of autoprotolysis constant $pK_{sp},$ negative logarithm (base 10) of solubility product

					Tempera	ture, °C				
Substance	0	5	10	15	20	25	30	35	40	50
Acetic acid (0)	4.780	4.770	4.762	4.758	4.757	4.756	4.757	4.762	4.769	4.787
DL-N-Acetylalanine (+1)		3.699	3.699	3.703	3.708	3.715	3.725	3.733	3.745	3.774
β -Acetylaminopropionic (+1)		4.479	4.465	4.465	4.449	4.445	4.444	4.443	4.445	4.457
<i>N</i> -Acetylglycine (+1)		3.682	3.676	3.673	3.667	3.670	3.673	3.678	3.685	3.706
α -Alanine										
(+1)	2.42		2.39		2.35	2.34	2.33	2.33	2.33	2.33
(0)	10.59		10.29		10.01	9.87	9.74	9.62	9.49	9.26
2-Aminobenzenesulfonic acid (0),										
pK_2	2.633	2.591	2.556	2.521	2.448	2.459	2.431	2.404	2.380	2.338
3-Aminobenzenesulfonic acid (0),										
pK_2	4.075	4.002	3.932	3.865	3.799	3.738	3.679	3.622	3.567	3.464
4-Aminobenzenesulfonic acid (0),										
pK_2	3.521	3.457	3.398	3.338	3.283	3.227	3.176	3.126	3.079	2.989
3-Aminobenzoic acid (0)					4.90	4.79	4.75		4.68	4.60
4-Aminobenzoic acid (0)					4.95	4.85	4.90		4.95	5.10
2-Aminobutyric acid										
(+1)			2.334			2.286		2.289 ^{37.5} °C		2.297
(0)			10.530			9.380		9.518 ^{37.5} °C		9.234
4-Aminobutyric acid										
(+1)			4.057	4.046	4.038	4.031	4.027	4.025	4.027	4.032
(0)			11.026	10.867	10.706	10.556	10.409	10.269	10.114	9.874
2-Aminoethylsulfonic acid (0)			9.452	9.316	9.186	9.061	8.940	8.824	8.712	9.499
2-Amino-3-methylpentanoic acid										
(+1)	2.365 ^{1 ℃}		2.338 ^{12.5} °C			2.320		2.317 ^{37.5} °C		2.332
(0)	10.460¹ °C		10.100 ^{12.5} °C			9.758		9.439 ^{37.5} °C	1	9.157

2-Amino-2-methyl-					I					
1,3-propanediol	9.612	9.433	9.266	9.104	8.951	8.801	8.659	8.519	8.385	8.132
2-Amino-2-methylpropionic acid										
(+1)	2.419¹° ^C		2.380 ^{12.5} °C			2.357		2.351 ^{37.5} °C		2.356
(0)	10.960 ^{1 °C}		10.580 ^{12.5} °C			10.205		$9.872^{37.5}$ °C		9.561
2-Aminopentanoic acid										
(+1)	2.376 ^{1 °C}		2.347			2.318			2.309	2.313
(0)	10.508 ^{1 °C}			10.154 ^{12.5} °C		9.808		9.490 ^{37.5} °C		9.198
3-Aminopropionic acid										
(+1)	3.656	3.627		3.583		3.551		3.524	3.517	
(0)	11.000	10.830		10.526		10.235		9.963	9.842	
4-Aminopyridine (+1)	9.873	9.704	9.549	9.398	9.252	9.114	8.978	8.846	8.717	8.477
Ammonium ion $(+1)$	10.081	9.904	9.731	9.564	9.400	9.425	9.093	8.947	8.805	8.539
Arginine										
(+1)	1.914	1.885	1.870	1.849	1.837	1.823	1.814	1.801	1.800	1.787
(0)	9.718	9.563	9.407	9.270	9.123	8.994	8.859	8.739	8.614	8.385
Barbituric acid										
(+1)				3.969	3.980	4.02	4.00	4.008	4.017	4.032
(0)				8.493	8.435	8.372	8.302	8.227	8.147	7.974
Benzoic acid (0)		4.231	4.220	4.215	4.206	4.204	4.203	4.207	4.219	4.223
Boric acid (0)	9.508	9.439	9.380	9.327	9.280	9.236	9.197	9.161	9.132	9.080
Bromoacetic acid (0)				2.875	2.887	2.902	2.918	2.936		
3-Bromobenzoic acid (0)				3.818	3.813	3.810	3.808	3.810	3.813	
4-Bromobenzoic acid (0)				4.011	4.005	3.99	4.001	4.001	4.003	
Bromopropynoic acid (0)			1.786	1.814	1.839	1.855	1.879	1.900	1.919	
3-tert-Butylbenzoic acid (0)				4.266	4.231	4.199	4.170	4.143	4.119	
4-tert-Butylbenzoic acid (0)				4.463	4.425	4.389	4.354	4.320	4.287	
2-Butynoic acid (0)			2.618	2.626	2.611	2.620	2.618	2.621	2.631	
Butyric acid (0)	4.806	4.804	4.803	4.805	4.810	4.817	4.827	4.840	4.854	4.885
DL-N-Carbamoylalanine (+1)		3.898	3.894	3.891	3.890	3.892	3.896	3.902	3.908	3.931
N-Carbamoylglycine (+1)		3.911	3.900	3.889	3.879	3.876	3.874	3.873	3.875	3.888

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*continued*)

	Temperature, °C										
Substance	0	5	10	15	20	25	30	35	40	50	
Carbon dioxide + water											
(0)	6.583	6.517	6.465	6.429	6.382	6.365	6.327	6.31	6.296	6.297	
(-1)	10.627	10.558	10.499	10.431	10.377	10.33	10.290	10.25	10.220	10.172	
Chloroacetic acid (0)				2.845	2.856	2.867	2.883	2.900			
3-Chlorobenzoic acid (0)				3.838	3.831	3.83	3.825	3.826	3.829		
4-Chlorobenzoic acid (0)				4.000	3.991	3.986	3.981	3.980	3.981		
Chloropropynoic acid (0)			1.766	1.796	1.820	1.845	1.864	1.879	1.893		
Citric acid											
(0)	3.220	3.200	3.176	3.160	3.142	3.128	3.116	3.109	3.099	3.095	
(-1)	4.837	4.813	4.797	4.782	4.769	4.761	4.755	4.751	4.750	4.757	
(-2)	6.393	6.386	6.383	6.384	6.388	6.396	6.406	6.423	6.439	6.484	
Cyanoacetic acid (0)		2.445	2.447	2.452	2.460	2.460	2.482	2.496	2.511		
2-Cyano-2-methylpropionic acid											
(0)		2.342	2.360	2.379	2.400	2.422	2.446	2.471	2.498		
5,5-Diethylbarbituric acid (0)	8.40	8.30	8.22	8.169	8.094	8.020	7.948	7.877	7.808	7.673	
Diethylmalonic acid											
(0)			2.129	2.136	2.144	2.151	2.160	2.172	2.187		
(-1)			7.400	7.401	7.408	7.417	7.428	7.441	7.457		
2,3-Dimethylbenzoic acid (0)				3.663	3.687	3.771	3.726	3.762	3.788		
2,4-Dimethylbenzoic acid (0)				4.154	4.187	4.217	4.244	4.268	4.290		
2,5-Dimethylbenzoic acid (0)				3.911	3.954	3.990	4.020	4.045	4.065		
2,6-Dimethylbenzoic acid (0)				3.234	3.304	3.362	3.409	3.445	3.472		
3,5-Dimethylbenzoic acid (0)				4.292	4.299	4.302	4.304	4.306	4.306		
<i>N</i> , <i>N</i> ′-Dimethylethyleneamine-											
N,N'-diacetic acid											
(0)	6.294		6.169		6.047		5.926		5.803		
(-1)	10.446		10.268		10.068		9.882		9.684		

N,N-Dimethylglycine (0)		10.34		10.14		9.94		9.76		
3,5-Dinitrobenzoic acid (0)			2.60		2.73		2.85		2.96	3.07
2-Ethylbutyric acid (0)	4.623		4.664		4.710	4.751	4.758		4.812	4.869
5-Ethyl-5-phenylbarbituric acid (0)				7.592	7.517	7.445	7.377	7.311	7.248	7.130
Fluoroacetic acid (0)				2.555	2.571	2.586	2.604	2.624		
Formic acid (0)	3.786	3.772	3.762	3.757	3.753	3.751	3.752	3.758	3.766	3.782
2-Furancarboxylic acid (0)						3.164	3.200	3.216	3.239	
Glucose-1-phosphate (0)		6.506	6.500	6.499	6.500	6.504	6.510	6.519	6.531	6.561
Glycerol-1-phosphoric acid (-1)		6.642	6.641	6.643	6.648	6.656	6.666	6.679	6.695	6.733
Glycerol-2-phosphoric acid										
(0)		1.223	1.245	1.271	1.301	1.335	1.372	1.413	1.457	1.554
(-1)		6.657	6.650	6.646	6.646	6.650	6.657	6.666	6.679	6.712
Glycine										
(+1)			2.397	2.380	2.36	2.351	2.34	2.33	2.327	2.32
(0)		10.34	10.193	10.044	9.91	9.780	9.65	9.53	9.412	9.19
Glycolic acid (0)	3.875		3.844 ^{12.5} °C			3.831		3.833 ^{37.5℃}		3.849
Glycylasparagine (+1)		2.968	2.958	2.952	2.943	2.942	2.942	2.944	2.947	2.959
N-Glycylglycine (+1)	3.201					3.126				3.159
			8.594 ^{12.5} °C			8.252		7.948 ^{37.5} °C		7.668
Hexanoic acid (0)	4.840		4.839		4.849		4.865		4.890	4.920
Hydrogen cyanide (0)			9.63	9.49	9.36	9.21	9.11	8.99	8.88	
Hydrogen peroxide (0)	12.23			11.86	11.75	11.65	11.55	11.45		11.21
Hydrogen sulfide										
(0)		7.33	7.24	7.13	7.05	6.97	6.90	6.82	6.79	6.69
(-1)		13.5		13.2		12.90	12.75	12.6		
4-Hydroxybenzoic acid (0)				4.596	4.586	4.582	4.577	4.576	4.578	
Hydroxylamine (0)				6.186	6.063	5.948		5.730		
2-Hydroxy-1-naphthoic acid										
(0)					3.29		3.24		3.19	3.26
(-1)					9.68		9.65		9.61	9.58
4-Hydroxyproline										
(+1)	1.900 ^{1 °C}		1.850 ^{12.5} °C			1.818		1.798 ^{37.5} °C		1.796
(0)	10.274 ^{1 °C}		9.95812.5℃			9.662		9.394 ^{37.5} °C		9.138
			ı.		1	1			1	1

 TABLE 8.3
 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (continued)

						Te	mperature, °C	C		
Substance	0	5	10	15	20	25	30	35	40	50
2-Hydroxypropionic acid (0)	3.880	3.873	3.868	3.861	3.857	3.858	3.861	3.867	3.873	3.895
DL-2-Hydroxysuccinic acid										
(0)	3.537	3.520	3.494	3.482	3.472	3.458	3.452	3.446	3.444	3.445
(-1)	5.119	5.108	5.098	5.096	5.096	5.097	5.099	5.104	5.117	5.149
Hypobromous acid (0)				8.83		8.60		8.47	8.37 ⁴⁵ ℃	
Hypochlorous acid (0)	7.82	7.75	7.69	7.63	7.58	7.54	7.50	7.46		7.05
Imidazole (+1)	7.581	7.467	7.334	7.216	7.103	6.993	6.887	6.784	6.685	6.497
Iodoacetic acid (0)				3.143	3.158	3.175	3.193	3.213		
DL-Isoleucine										
(+1)	2.365		2.338 ^{12.5} °C			2.318		2.317 ^{37.5} ℃		2.332
(0)	10.460		10.100 ^{12.5} °C			9.758		9.439 ^{37.5} °C		9.157
Isopropylmalonic acid,										
mononitrile (0)		2.299	2.320	2.343	2.365	2.401	2.427	2.452	2.481	
Lactic acid (0)	3.880	3.873	3.868	3.862	3.857	3.858	3.861	3.867	3.873	3.895
Lead sulfate, pK _{sp}	8.01			7.87		7.80		7.73		7.63
DL-Leucine										
(+1)	2.3831°C		2.348 ^{12.5} °C			2.328		2.327 ^{37.5} °C		2.333
(0)	10.458 ^{1 °C}		10.095 ^{1.5} °C			9.744		9.434 ^{37.5} °C		9.142
Malonic acid (−1)	5.670	5.665	5.667	5.673	5.683	5.696	5.710	5.730	5.753	5.803
Mannose (0)			12.45			12.08			11.81	
Mercury(I) chloride, pK _{sp}			18.65	18.48	18.27	17.88		16.79		
Methanol (solvent), pK _{auto}		17.12		16.84		16.71	16.65	16.53		
Methylamine (+1)	11.496		11.130		10.787	10.62	10.466		10.161	9.876
Methylaminodiacetic acid										
(0)	2.138		2.142		2.146		2.150		2.154	
(-1)	10.474		10.287		10.088		9.920		9.763	

3-Methylbenzoic acid (0) 4-Methylbenzoic acid (0)				4.303 4.390	4.285 4.376	4.269 4.362	4.256 4.349	4.244 4.336	4.235	
3-Methylbutyric acid (0)	4.726		4.742	4.390	4.767	4.302	4.794	4.550	4.831	4.871
4-Methylpentanoic acid (0)	4.720		4.827		4.837		4.853		4.879	4.908
5-Methyl-5-phenylbarbituric acid	4.027		4.627		4.657		4.033		4.079	4.900
(0)				8.104	8.057	8.011	7.966	7.922	7.879	7.797
2-Methylpropionic acid (0)	4.825		4.827	0.104	4.840	4.853	4.886	1.922	4.918	4.955
2-Methyl-2-propylamine (+1)	4.023	11.439	11.240	11.048	10.862	10.682	10.511	10.341	4.910	4.933
Nitric acid (0)	-1.65	11.439	11.240	11.046	10.602	-1.38	10.511	10.541		-1.20
Nitrilotriacetic acid	1.03					1.36				1.20
(0)	1.69		1.65		1.65		1.66		1.67	
(-1)	2.95		2.95		2.94		2.96		2.98	
(-1) (-2)	10.59		10.45		10.33		10.23		2.90	
4-Nitrobenzoic acid (0)	10.39		10.43	3.448	3.444	3.441	3.441	3.442	3.445	
Nitrous acid (0)				3.244	3.177	3.138	3.441	3.100	3.443	
DL-Norleucine				3.244	3.177	3.136		3.100		
(+1)	2.394		2.356 ^{12.5°C}			2.335		2.324 ^{37.5} °C		2.328
(0)	10.564		10.190 ^{12.5} °C			9.834		9.513 ^{37.5} °C		9.224
Oxalic acid (-1)	4.210	4.216	4.227	4.240	4.254	4.272	4.295	4.318	4.349	4.409
2,4-Pentanedione (0)	9.07	4.210	4.227	4.240	4.234	8.95	4.293	4.310	8.90	4.409
Pentanoic acid (0)	4.823		4.763		4.835	4.842	4.851		4.861	4.906
Phenylalanine (0)	4.023		9.75		4.655	9.31	4.031		8.96	4.900
Phosphoric acid (0)	2.056	2.073	2.088	2.107	2.127	2.148	2.171	2.196	2.224	2.277
(-1)	7.313	7.282	7.254	7.231	7.213	7.198	7.189	7.185	7.181	7.183
o-Phthalic acid	7.313	1.262	7.234	7.231	7.213	7.196	7.109	7.103	7.101	7.103
(0)	2.925	2.927	2.931	2.937	2.943	2.950	2.958	2.967	2.978	3.001
(-1)	5.432	5.418	5.410	5.405	5.405	5.408	5.416	5.427	5.442	5.485
Piperidine (+1)	11.963	11.786	11.613	11.443	11.280	11.123	10.974	10.818	10.670	10.384
Proline	11.903	11.760	11.013	11.443	11.260	11.123	10.574	10.616	10.070	10.564
(+1)	2.011		1.964 ^{12.5} °C			1.952		1.950 ^{37.5} °C		1.958
(0)	11.296		1.904 10.972 ^{12.5} °C			1.932		1.930°10.342 ^{37.5} °C	10.064	1.930
(0)	11.290		10.972	1	I	10.040		10.342	10.004	

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (continued)

		Temperature, °C											
Substance	0	5	10	15	20	25	30	35	40	50			
Propenoic acid (0)				4.267	4.250	4.247	4.249	4.267	4.301				
<i>N</i> -Propionylglycine (+1)		3.728	3.723	3.718	3.716	3.718	3.721	3.725	3.731	3.750			
Propynoic acid (0)			1.791	1.829	1.867	1.887	1.940	1.932	1.963				
Pyrrolidine (+1)	12.17	11.98	11.81	11.63	11.43	11.30	11.15	10.99	10.84	11.56			
Serine													
(+1)	2.2961°C		2.232 ^{12.5} ℃			2.186		2.154 ^{37.5} °C		2.132			
(0)	9.880 ¹ °C		9.54212.5℃			9.208		8.904 ^{37.5} °C		8.628			
Silver bromide, pK _{sp}		13.33		12.83	12.57	12.30	12.07	11.83	11.61	11.19			
Silver chloride, pK _{sp}		10.595		10.152		9.749		9.381	9.21	8.88			
Succinic acid													
(0)	4.285	4.263	4.245	4.232	4.218	4.207	4.198	4.191	4.188	4.186			
(-1)	5.674	5.660	5.649	5.642	5.639	5.635	6.541	5.647	5.654	5.680			
Sulfuric acid (-1)	1.778	1.812 ^{4.3} °C		1.894		1.987	2.05	2.095	2.17	2.246			
Sulfurous acid (0)	1.63		1.74			1.89		1.98		2.12			
D-Tartaric acid													
(0)	3.118	3.095	3.075	3.057	3.044	3.036	3.025	3.019	3.018	3.021			
(-1)	4.426	4.407	4.391	4.381	4.372	4.366	4.365	4.367	4.372	4.391			
2,3,5,6-Tetramethylbenzoic acid (0)				3.310	3.367	3.415	3.453	3.483	3.505				
Threonine													
(+1)	2.200 ^{1 °C}		2.132 ^{12.5} ℃			2.088		2.070 ^{37.5} °C		2.055			
(0)	9.748 ^{1℃}		9.42012.5℃			9.100		8.812 ^{37.5} °C		8.548			
o-Toluidine (0)				4.58	4.495	4.45	4.345	4.28	4.20				
1,2,4-Triazole													
(+1)				2.451	2.418	2.386	2.327						
(0)				10.205	10.083	9.972	9.768						
3,4,5-Trihydroxybenzoic acid (0)					4.19		4.30		4.38	4.53			

Tris(2-hydroxyethyl)amine (+1)	8.290	8.173	8.067	7.963	7.861	7.762	7.666	7.570	7.477	7.299
2,4,6-Trimethylbenzoic acid (0)				3.325	3.391	3.448	3.498	3.541	3.577	
3-Trimethylsilylbenzene acid (0)				4.142	4.116	4.089	4.060	4.029	3.996	
4-Trimethylsilylbenzoic acid (0)				4.270	4.230	4.192	4.155	4.119	4.084	
β -Ureidopropionic acid (0)		4.514	4.505	4.497	4.490	4.487	4.486	4.486	4.488	4.500
DL-Valine										
(+1)	2.320		2.297 ^{12.5} °C			2.296		2.292 ^{37.5} °C		2.310
(0)	10.413		10.064 ^{12.5} °C			9.719		9.405 ^{37.5} °C		9.124

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TABLE 8.4 Indicators for Aqueous Acid–Base Titrations

Table 8.4 lists selected common indicators. The table is arranged according to function over increasing pH range or transition interval given (third column). Note that this range may vary appreciably from one observer to another, and that it is also affected by ionic strength, temperature, and illumination. The values given should therefore be considered to be approximate. These values refer to solutions having low ionic strengths and a temperature of about 25 °C. In the fourth column the pK_A ($-\log K_A$) of the indicator as determined spectrophotometrically is listed. In the fifth and sixth columns, the wavelength of maximum absorption is given for the acidic and basic forms of the indicator, respectively. The lower to higher pH color change is given in the last column. The abbreviations used to describe the colors of the two forms of the indicator are as follows:

B, Blue P, Purple
C, Colorless R, Red
G, Green V, Violet
O, Orange Y, Yellow

OBr, Orange-brown

				λ_{\max}	, nm	- Color
Indicator	Chemical name	pH range	pK _A	Acid	Base	change
Cresol red	o-Cresolsulfonephthalein	0.2–18				R-Y
(acid range)						
Cresol purple (acid range)	<i>m</i> -Cresolsulfonephthalein	1.2–2.8	1.51	533		R–Y
Thymol blue (acid range)	Thymolsulfonephthalein	1.2–2.8	1.65	544	430	R–Y
Tropeolin OO	Diphenylamino- <i>p</i> -benzene sodium sulfonate	1.3–3.2	2.0	527		R–Y
2,6-Dinitrophenol	2,6-Dinitrophenol	2.4-4.0	3.69			C-Y
2,4-Dinitrophenol	2,4-Dinitrophenol	2.5-4.3	3.90			C-Y
Methyl yellow	Dimethylaminoazobenzene	2.9-4.0	3.3	508		R-Y
Methyl orange	Dimethylaminoazobenzene sodium sulfonate	3.1–4.4	3.40	522	464	R–O
Bromophenol blue	Tetrabromophenolsulfonephthalein	3.0-4.6	3.85	436	592	Y–BV
Bromocresol green	Tetrabromo- <i>m</i> -cresol-sulfonephthalein	4.0–5.6	4.68	444	617	Ү–В
Methyl red	o-Carboxybenzeneazo- dimethylaniline	4.4–6.2	4.95	530	427	R-Y
Chlorophenol red	Dichlorophenolsulfonephthalein	5.4-6.8	6.0		573	Y-R
Bromocresol purple	Dibromo-o-cresolsulfonephthalein	5.2-6.8	6.3	433	591	Y–P
Bromophenol red	Dibromophenolsulfonephthalein	5.2-6.8			574	Y-R
<i>p</i> -Nitrophenol	<i>p</i> -Nitrophenol	5.3-7.6	7.15	320	405	C-Y
Bromothymol blue	Dibromothymolsulfonephthalein	6.2–7.6	7.1	433	617	Ү–В
Neutral red	Aminodimethylaminotoluphen- azonium chloride	6.8–8.0	7.4			R–Y
Phenol red	Phenolsulfonephthalein	6.4-8.0	7.9	433	558	Y-R

TABLE 8.4 Indicators for Aqueous Acid–base Titrations (*continued*)

				λ_{max}	, nm	Color
Indicator	Chemical name	pH range	pK_A	Acid	Base	change
<i>m</i> -Nitrophenol	<i>m</i> -Nitrophenol	6.4–8.8	8.3		570	C-Y
Cresol red	o-Cresolsulfonephthalein	7.2-8.8	8.2	434	572	Y–R
m-Cresol purple	<i>m</i> -Cresolsulfonephthalein	7.6–9.2	8.32		580	Y-P
Thymol blue	Thymolsulfonephthalein	8.0-9.6	8.9	430	596	Y–B
Phenolphthalein	Phenolphthalein	8.0-10.0	9.4		553	C-R
α -Naphtholbenzein	α-Naphtholbenzein	9.0–11.0				Ү–В
Thymolphthalein	Thymolphthalein	9.4–10.6	10.0		598	С-В
Alizarin yellow	5-(p-Nitrophenylazo)salicylic acid, Na salt	10.0–12.0	11.16			Y–V
Tropeolin O	<i>p</i> -Sulfobenzeneazoresorcinol	11.0-13.0				Y-OBr
Nitramine	2,4,6-Trinitrophenyl- methylnitroamine	10.8–13.0				C–OBr

 TABLE 8.5
 National Institute of Standards and Technology (formerly National Bureau of Standards U.S). Reference PH Buffer Solutions.

Temperature °C	Secondary standard 0.05 M Potassium tetraoxalate	Potassium hydrogen tartrate (saturated at 25 °C)	0.05 M Potassium dihydrogen citrate	0.05 M Potassium hydrogen phthalate	$0.025\mathrm{M} \\ \mathrm{KH_2PO_4}, \\ 0.025\mathrm{M} \\ \mathrm{Na_2HPO_4}$	0.0087 M KH ₂ PO ₄ , 0.0302 M Na ₂ HPO ₄	$\begin{array}{c} 0.01\mathrm{M} \\ \mathrm{Na_2B_4O_7} \end{array}$	0.025 M NaHCO ₃ , 0.025 M Na ₂ CO ₃	Secondary standard Ca(OH) ₂ (saturated at 25°C)
0	1.666		3.860	4.003	6.984	7.534	9.464	10.317	13.423
5	1.668		3.840	3.999	6.951	7.500	9.395	10.245	13.207
10	1.670		3.820	3.998	6.923	7.472	9.332	10.179	13.003
15	1.672		3.802	3.999	6.900	7.448	9.276	10.118	12.810
20	1.675		3.788	4.002	6.881	7.429	9.225	10.062	12.627
25	1.679	3.557	3.776	4.008	6.865	7.413	9.180	10.012	12.454
30	1.683	3.552	3.766	4.015	6.853	7.400	9.139	9.966	12.289
35	1.688	3.549	3.759	4.024	6.844	7.389	9.102	9.925	12.133
38	1.691	3.548		4.030	6.840	7.384	9.081		12.043
40	1.694	3.547	3.753	4.035	6.838	7.380	9.068	9.889	11.984
45	1.700	3.547		4.047	6.834	7.373	9.038		11.841
50	1.707	3.549	3.749	4.060	6.833	7.367	9.011	9.828	11.705
55	1.715	3.554		4.075	6.834		8.985		11.574
60	1.723	3.560		4.091	6.836		8.962		11.449
70	1.743	3.580		4.126	6.845		8.921		
80	1.766	3.609		4.164	6.859		8.885		
90	1.792	3.650		4.205	6.877		8.850		
95	1.806	3.674		4.227	6.886		8.833		
Dilution value $\Delta pH_{1/2}$	+0.186	+0.049	0.024	+0.052	+0.080	+0.070	+0.01	0.079	-0.28

Source: R. G. Bates, J. Res. Natl. Bur. Stand. (U.S.), 66A:179 (1962) and B. R. Staples and R. G. Bates, ibid, 73A: 37 (1969).

TABLE 8.6 Compositions of National Institute of Standards and Technology. Standard pH Buffer Solutions

Air weight of material per liter of buffer solution

Standard	Weight, g
$KH_3(C_2O_4)_2 \cdot 2H_2O, 0.05 M$	12.61
Potassium hydrogen tartrate, about 0.034M	Saturated at 25 °C
Potassium hydrogen phthalate, 0.05 M	10.12
Phosphate (solution 1)	
KH_2PO_4 , 0.025 M	3.39
Na_2HPO_4 , 0.025 M	3.53
Phosphate (solution 2)	
KH_2PO_4 , 0.008665 M	1.179
Na_2HPO_4 , 0.03032 M	4.30
$Na_2B_4O_7 \cdot 10H_2O, 0.01 M$	3.80
Carbonate	
NaHCO ₃ , 0.025 M	2.10
Na_2CO_3 , 0.025 M	2.65
$Ca(OH)_2$, about $0.0203 M$	Saturated at 25 °C

Standard Reference pH Buffer Solutions

The buffer value for the National Institute of Standards and technology (U.S.) reference pH buffer solutions is given below:

Buffer solution	KH tartrate	0.05 M KH ₂ citrate	0.05 M KH phthalate	$0.025\mathrm{M}$ $\mathrm{KH_2PO_4},$ $0.025\mathrm{M}$ $\mathrm{Na_2HPO_4}$	$0.0087\mathrm{M}$ $\mathrm{KH_2PO_4},$ $0.0302\mathrm{M}$ $\mathrm{Na_2HPO_4}$	0.01 M Na ₂ B ₄ O ₇	0.025 M NaHCO ₃ , 0.025 M Na ₂ CO ₃
Buffer value β	0.027	0.034	0.016	0.029	0.016	0.020	0.029

For the secondary pH reference standards, the buffer value is 0.070 for potassium tetraoxalate and 0.09 for calcium hydroxide.

To prepare the standard pH buffer solutions recommended by the National Bureau of Standards (U.S.), the indicated weights of the pure materials in Table 8.6 should be dissolved in water of specific conductivity not greater than 5 micromhos. The tartrate, phthalate, and phosphates can be dried for 2h at 110 °C before use. Potassium tetraoxalate and calcium hydroxide need not be dried. Fresh-looking crystals of borax should be used. Before use, excess solid potassium hydrogen tartrate and calcium hydroxide must be removed. Buffer solutions pH 6 or above should be stored in plastic containers and should be protected from carbon dioxide with soda-lime traps. The solutions should be replaced

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within 2 to 3 weeks, or sooner if formation of mold is noticed. A crystal of thymol may be added as a preservative.

Buffer Solutions other than Standards

The range of the buffering effect of a single weak acid group is approximately one pH unit on either side of the pK_A . The ranges of some useful buffer systems are collected in Table 8.7. After all the components have been brought together, the pH of the resulting solution should be determined at the temperature to be employed with reference to standard reference solutions. Buffer components should be compatible with other components in the system under study; this is particularly significant for buffers employed in biological studies. Check tables of formation constants to ascertain whether metal-binding character exists.

When there are two or more acid groups per molecule, or a mixture is composed of several overlapping acids, the useful range is larger. Universal buffer solutions consist of a mixture of acid groups which overlap such that successive pK_A values differ by 2 pH units or less. The Prideaux–Ward mixture comprises phosphate, phenyl acetate, and borate plus HCl and covers the range from 2 to 12 pH units. The McIlvaine buffer is a mixture of citric acid and Na₂HPO₄ that covers the range from pH 2.2 to 8.0. The Britton–Robinson system consists of acetic acid, phosphoric acid, and boric acid plus NaOH and covers the range from pH 4.0 to 11.5. A mixture composed of Na₂CO₃, NaH₂PO₄, citric acid, and 2-amino-2-methyl-1.3-propanediol covers the range from pH 2.2 to 11.0.

TABLE 8.7 pH Values of Buffer Solutions for Control Purposes

Materials*	pH range
Glycine and HCl	1.0-3.7
Citrate and HCl	1.3-4.7
<i>p</i> -Toluenesulfonate and <i>p</i> -toluenesulfonic acid	1.1-3.3
Formate and HCl	2.8-4.6
Succinic acid and borax	3.0-5.8
Phenyl acetate and HCl	3.5-5.0
Acetate and acetic acid	3.7–5.6
Succinate and succinic acid	4.8-6.3
2-(N-Morpholino)ethanesulfonic acid and NaOH	5.2–7.1
2,2-Bis(hydroxymethyl)-2,2',2"-nitrilotriethanol and HCl	5.8-7.2
KH ₂ PO ₄ and borax	5.8-9.2
N-Tris(hydroxymethyl)methyl-2-aminoethanesulfonic acid and NaOH	6.8-8.2
KH ₂ PO ₄ and Na ₂ HPO ₄	6.1–7.5
N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid and NaOH	6.9-8.3
Triethanolamine and HCl	6.9-8.5
Diethylbarbiturate (veronal) and HCl	7.0-8.5
Tris(hydroxymethyl)aminomethane and HCl	7.2–9.0
N-Tris(hydroxymethyl)methylglycine and HCl	
<i>N,N</i> -Bis(2-hydroxyethyl)glycine and HCl	
Borax and HCl	7.6-8.9
Glycine and NaOH	8.2-10.1
Ammonia (aqueous) and NH ₄ Cl	8.3-9.2
Ethanolamine and HCl	8.6–10.4

Borax and NaOH	9.4–11.1
Carbonate and hydrogen carbonate	9.2-11.0
Na ₂ HPO ₄ and NaOH	11.0–12.0

General directions for the preparation of buffer solutions of varying pH but fixed ionic strength are given by Bates.* Preparation of McIlvaine buffered solutions at ionic strengths of 0.5 and 1.0 and Britton–Robinson solutions of constant ionic strength have been described by Elving et al.† and Frugoni,‡ respectively.

REFERENCE ELECTRODES

TABLE 8.8 Potentials of Reference Electrodes (in volts) as a Function of Temperature

Liquid-junction potential included

Temp., °C	0.1 M KCl, calomel*	1.0 M KCl, calomel*	3.5 M KCl, calomel*	Saturated KCl, calomel*	1.0M KCl, Ag/AgCl†	1.0M KBr, Ag/AgBr‡	1.0M KI, Ag/AgI§
0	0.3367	0.2883		0.25918	0.23655	0.08128	-0.14637
5					0.23413	0.07961	-0.14719
10	0.3362	0.2868	0.2556	0.25387	0.23142	0.07773	-0.14822
15	0.3361			0.2511	0.22857	0.07572	-0.14942
20	0.3358	0.2844	0.2520	0.24775	0.22557	0.07349	-0.15081
25	0.3356	0.2830	0.2501	0.24453	0.22234	0.07106	-0.15244
30	0.3354	0.2815	0.2481	0.24118	0.21904	0.06856	-0.15405
35	0.3351			0.2376	0.21565	0.06585	-0.15590
38	0.3350		0.2448	0.2355			
40	0.3345	0.2782	0.2439	0.23449	0.21208	0.06310	-0.15788
45					0.20835	0.06012	-0.15998
50	0.3315	0.2745		0.22737	0.20449	0.05704	-0.16219
55					0.20056		
60	0.3248	0.2702		0.2235	0.19649		
70					0.18782		
80				0.2083	0.1787		
90					0.1695	0.0251	

^{*} Bates et al., J. Res. Natl. Bur. Stand., 45:418 (1950).

[§] Hetzer, Robinson, and Bates, J. Phys. Chem., 68:1929 (1964).

Temp., °C	125	150	175	200	225	250	275
1.0 M KCl, Ag/AgCl*	0.1330	0.1032	0.0708	0.0348	-0.0051	-0.054	-0.090
1.0 M KBr, Ag/AgBr†	-0.0048	-0.0312	-0.0612	-0.0951			

^{*} Greeley et al., J. Phys. Chem., 64:652 (1960).

^{*} Bates, Determination of pH, Theory and Practice, Wiley, New York, 1964, pp. 121–122.

[†] Elving, Markowitz, and Rosenthal, Anal. Chem., 28:1179 (1956).

[‡] Frugoni, Gazz. Chim. Ital., 87:403 (1957).

[†] Bates and Bower, J. Res. Natl. Bur. Stand., 53:283 (1954).

[‡] Hetzer, Robinson, and Bates, J. Phys. Chem., 66:1423 (1962).

[†] Towns et al., J. Phys. Chem., 64:1861 (1960).

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The values of several additional reference electrodes at 25 °C are listed:

Reference electrode	Potential, V
Ag/AgCl, saturated KCl	0.198
Ag/AgCl, 0.1 M KCl	0.288
Hg/HgO, 1.0 M NaOH	0.140
Hg/HgO, 0.1 M NaOH	0.165
Hg/Hg ₂ SO ₄ , saturated K ₂ SO ₄ (22°C)	0.658
Hg/HgSO ₄ , saturated KCl	0.655

TABLE 8.9 Potentials of Reference Electrodes (in volts) at $25\,^{\circ}$ C for water–organic solvent mixtures *Electrolyte solution of 1 M HCl*

Solvent, wt %	Methanol, Ag/AgCl	Ethanol, Ag/AgCl	2-Propanol, Ag/AgCl	Acetone, Ag/AgCl	Dioxane, Ag/AgCl	Ethylene glycol, Ag/AgCl	Methanol, calomel	Dioxane, calomel
5			0.2180	0.2190		0.2190		
10	0.2153	0.2146	0.2138	0.2156		0.2160		
20	0.2090	0.2075	0.2063	0.2079	0.2031	0.2101	0.255	0.2501
30		0.2003				0.2036		
40	0.1968	0.1945		0.1859		0.1972	0.243	
45					0.1635			0.2104
50		0.1859		0.158				
60	0.1818	0.173				0.1807		
70		0.158			0.0659		0.216	0.1126
80	0.1492	0.136						
82					-0.0614			-0.0014
90	0.1135	0.196		-0.034				
94.2	0.0841							
98		0.0215						
99							0.103	
100	-0.0099	-0.0081		-0.53				

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ELECTRODE POTENTIALS

TABLE 8.10 Potentials of Selected Half-Reactions at 25 °C

This table is a summary of oxidation-reduction half-reactions arranged in order of decreasing oxidation strength and is useful for selecting reagent systems.

Abbreviations Used in the Table g, gas liq, liquid s, solid

Half-reac	E° , V	
$F_2(g) + 2H^+ + 2e^-$	= 2HF	3.06
$O_3 + 2H^+ + 2e^-$	$= O_2 + H_2O$	2.07
$S_2O_8^{2-} + 2e^-$	$=2SO_4^{2-}$	2.01
$Ag^{2+} + e^{-}$	$=Ag^+$	2.00
$H_2O_2 + 2H^+ + 2e^-$	$= 2H_2O$	1.77
$MnO_4^- + 4H^+ + 3e^-$	$= MnO_2(s) + 2H_2O$	1.70
$Ce(IV) + e^{-}$	= Ce(III) (in 1 M HClO ₄)	1.61
$H_5IO_6 + H^+ + 2e^-$	$= IO_3^- + 3H_2O$	1.6
Bi_2O_4 (bismuthate) + $4H^+ + 2e^-$	$= 2BiO^+ + 2H_2O$	1.59
$BrO_3^- + 6H^+ + 5e^-$	$=\frac{1}{2}Br_2 + 3H_2O$	1.52
$MnO_4^- + 8H^+ + 5e^-$	$=Mn^{2+}+4H_2O$	1.51
$PbO_2 + 4H^+ + 2e^-$	$= Pb^{2+} + 2H_2O$	1.455
$Cl_2 + 2e^-$	$=2C1^{-}$	1.36
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6e^-$	$=2Cr^{3+}+7H_2O$	1.33
$MnO_2(s) + 4H^+ + 2e^-$	$= Mn^{2+} + 2H_2O$	1.23
$O_2(g) + 4H^+ + 4e^-$	$=2H_2O$	1.229
$IO_3^- + 6H^+ + 5e^-$	$=\frac{1}{2}I_2 + 3H_2O$	1.20
$Br_2(liq) + 2e^-$	$=2\mathrm{Br}^{-}$	1.065
$ICl_2^2 + e^-$	$=\frac{1}{2}I_2 + 2Cl^-$	1.06
$VO_2^+ + 2H^+ + e^-$	$=VO^{2+} + H_2O$	1.00
$HNO_2 + H^+ + e^-$	$= NO(g) + H_2O$	1.00
$NO_3^- + 3H^+ + 2e^-$	$= HNO_2 + H_2O$	0.94
$2Hg^{2+} + 2e^{-}$	$= Hg_2^{2+}$	0.92
$Cu^{2+} + I^{-} + e^{-}$	= CuI	0.86
$Ag^+ + e^-$	= Ag	0.799
$Hg_2^{2+} + 2e^-$	= 2Hg	0.79
$Fe(III) + e^-$	$= Fe^{2+}$	0.771
$O_2(g) + 2H^+ + 2e^-$	$= H_2O_2$	0.682
$2\text{HgCl}_2 + 2e^-$	$= Hg_2Cl_2(s) + 2Cl^-$	0.63
$Hg_2SO_4(s) + 2e^-$	$= 2Hg + SO_4^{2-}$	0.615
$H_3AsO_4 + 2H^+ + 2e^-$	$= HAsO_2 + 2H_2O$	0.581
$Sb_2O_5 + 6H^+ + 4e^-$	$= 2SbO^{+} + 3H_{2}O$	0.559
$I_3^- + 2e^-$	= 3I ⁻	0.545
$Cu^+ + e^-$	= Cu	0.52
$VO^{2+} + 2H^+ + e^-$	$= V^{3+} + H_2O$	0.337
$Fe(CN)_6^{3-} + e^{-}$	$= \operatorname{Fe}(\operatorname{CN})_{6}^{4-}$	0.36
$Cu^{2+} + 2e^{-}$	= Cu	0.337
$UO_2^{2+} + 4H^+ + 2e^-$	$= U^{4+} + 2H_2O$	0.334
$BiO^{+} + 2H^{+} + 3e^{-}$	= Bi + H2O	0.32
$Hg_2Cl_2(s) + 2e^-$	$= 2Hg + 2C1^{-}$	0.2676
$AgCl(s) + e^{-}$	$= Ag + Cl^{-}$	0.2223

TABLE 8.10 Potentials of Selected Half-Reactions at 25 °C (*continued*)

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Ha	If-reaction	E°, V
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$SbO^{+} + 2H^{+} + 3e^{-}$	$= Sb + H_2O$	0.212
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$= Cu + 3Cl^{-}$	0.178
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$SO_4^{2-} + 4H^+ + 2e^-$	$= SO_2(aq) + 2H_2O$	0.17
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Sn^{4+} + 2e^{+}$		0.154
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$S + 2H^+ + 2e^-$	$= H_2S(g)$	0.141
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$TiO^{2+} + 2H^+ + e^-$		0.10
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$S_4O_6^{2-} + 2e^-$	$=2S_2O_3^{2-}$	0.08
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$AgBr(s) + e^{-}$	$= Ag + Br^{-}$	0.071
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$2H^+ + 2e^-$		0.0000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		= Pb	-0.126
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$\mathrm{Sn}^{2+} + 2e^{-}$	= Sn	-0.136
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$AgI(s) + e^{-}$	$= Ag + I^-$	-0.152
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Mo^{3+} + 3e^-$	= Mo	ca-0.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$N_2 + 5H^+ + 4e^-$	$= H_2NNH_3^+$	-0.23
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Ni^{2+} + 2e^{-}$	= Ni	-0.246
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$V^{3+} + e^-$	$= V^{2+}$	-0.255
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\text{Co}^{2+} + 2e^{-}$	= Co	-0.277
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Ag(CN)_{2}^{-} + e^{-}$	$= Ag + 2CN^-$	-0.31
$\begin{array}{llllllllllllllllllllllllllllllllllll$		•	-0.403
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Cr^{3+} + e^{-}$	$= Cr^{2+}$	-0.41
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Fe^{2+} + 2e^{-}$	= Fe	-0.440
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$2\text{CO}_2 + 2\text{H}^+ + 2e^-$	$= H_2C_2O_4$	-0.49
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			-0.50
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			-0.61
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Zn^{2+} + 2e^-$	= Zn	-0.763
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Cr^{2+} + 2e^{-}$	= Cr	-0.91
$\begin{array}{lllll} Ti^{3+} + 3e^{-} & = Ti & -1.63 \\ Al^{3+} + 3e^{-} & = Al & -1.66 \\ Th^{4+} + 4e^{-} & = Th & -1.90 \\ Mg^{2+} + 2e^{-} & = Mg & -2.37 \\ La^{3+} + 3e^{-} & = La & -2.52 \\ Na^{+} + e^{-} & = Na & -2.714 \\ Ca^{2+} + 2e^{-} & = Ca & -2.870 \\ Sr^{2+} + 2e^{-} & = Sr & -2.89 \\ K^{+} + e^{-} & = K & -2.925 \\ \end{array}$	$Mn^{2+} + 2e^-$	= Mn	-1.18
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Zr^{4+} + 4e^{-}$	= Zr	-1.53
$\begin{array}{lllll} Th^{4+} + 4e^- & = Th & -1.90 \\ Mg^{2+} + 2e^- & = Mg & -2.37 \\ La^{3+} + 3e^- & = La & -2.52 \\ Na^+ + e^- & = Na & -2.714 \\ Ca^{2+} + 2e^- & = Ca & -2.870 \\ Sr^{2+} + 2e^- & = Sr & -2.89 \\ K^+ + e^- & = K & -2.925 \\ \end{array}$	$Ti^{3+} + 3e^-$	= Ti	-1.63
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Al^{3+} + 3e^{-}$	= A1	- 1.66
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Th^{4+} + 4e^{-}$		
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Mg^{2+} + 2e^{-}$	= Mg	-2.37
$egin{array}{lll} Na^+ + e^- & = Na & -2.714 \\ Ca^{2^+} + 2e^- & = Ca & -2.870 \\ Sr^{2^+} + 2e^- & = Sr & -2.89 \\ K^+ + e^- & = K & -2.925 \\ \end{array}$	$La^{3+} + 3e^{-}$		
$\begin{array}{ccccccc} {\rm Ca}^{2^+} + 2e^- & = {\rm Ca} & -2.870 \\ {\rm Sr}^{2^+} + 2e^- & = {\rm Sr} & -2.89 \\ {\rm K}^+ + e^- & = {\rm K} & -2.925 \end{array}$			-2.714
$Sr^{2^+} + 2e^-$ = Sr -2.89 $K^+ + e^-$ = K -2.925			
$K^+ + e^- = K$ -2.925			
$L_1' + e = L_1$ = -3.045	$\operatorname{Li}^+ + e^-$	= Li	-3.045

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25 °C

The solvent systems in this table are listed below:

- A, acetonitrile and a perchlorate salt such as LiClO₄ or a tetraalkyl ammonium salt
- B, acetic acid and an alkali acetate, often plus a tetraalkyl ammonium iodide
- C, 0.05 to 0.175 M tetraalkyl ammonium halide and 75% 1,4-dioxane
- D, buffer plus 50% ethanol (EtOH)

Abbreviations Used in the Table

Bu, butyl M, molar MeOH, methanol Et, ethyl Me, methyl PrOH, propanol EtOH, ethanol

Compound Solvent system $E_{1/2}$ Unsaturated aliphatic hydrocarbons Acrylonitrile C but 30% EtOH -1.94Allene C -2.291.3-Butadiene Α -2.03C -2.591,3-Butadiyne C -1.891-Buten-2-yne C -2.401,4-Cyclohexadiene Α -1.6Cyclohexene Α -1.891,3,5,7-Cyclooctatetraene В -1.42C-1.51Diethyl fumarate B, pH 4.0 -0.84Diethyl maleate B, pH 4.0 -0.952,3-Dimethyl-1,3-butadiene -1.83Dimethylfulvene C -1.89Diphenylacetylene \mathbf{C} -2.201,1-Diphenylethylene В -1.52C -2.19Ethyl methacrylate 0.1 N LiCl + 25% EtOH -1.92-Methyl-1,3-butadiene -1.842-Methyl-1-butene A -1.971-Piperidino-4-cyano-4-phenyl-1.3-butadiene LiClO₄ in dimethylformamide -0.16trans-Stilbene В -1.51Tetrakis(dimethylamino)ethylene Α -0.75Aromatic hydrocarbons Acenaphthene Α -0.95В -1.36C -2.58Anthracene Α -0.84В -1.20C -1.94

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$
	Aromatic hydrocarbons (continued)	
Azulene	A	-0.71
	C	-1.66, -2.26,
		-2.56
1,2-Benzanthracene	C	-2.03, -2.54
2,3-Benzanthracene	A	-0.54, -1.20
Benzene	A	-2.08
1,2-Benzo[a]pyrene	A	-0.76
Biphenyl	A	-1.48
	В	-1.91
	C	-2.70
Chrysene	A	-1.22
1,2,5,6-Dibenzanthracene	A	-1.00, -1.26
1,2-Dihydronaphthalene	C	-2.57
9,10-Dimethylanthracene	A	-0.65
2,3-Dimethylnaphthalene	A	-1.08, -1.34
9,10-Diphenylanthracene	A	-0.92
Fluorene	A	-1.25
	В	-1.65
	C	-2.65
Hexamethylbenzene	A	-1.16
	В	-1.52
Indan	A	-1.59, -2.02
Indene	A	-1.23
	C	-2.81
1-Methylnaphthalene	A	-1.24
	В	-1.53
	C	-2.46
2-Methylnaphthalene	A	-1.22
	В	-1.55
	C	-2.46
Naphthalene	A	-1.34
	В	-1.72
Pentamethylbenzene	A	-1.28
•	В	-1.62
Phenanthrene	A	-1.23
	В	-1.68
	C	-2.46, -2.71
Phenylacetylene	C	-2.37
Pyrene	A	-1.06, -1.24
trans-Stilbene	В	-1.51
	C	-2.26
Styrene	C	-2.35
1,2,3,5-Tetramethylbenzene	A	-1.50, -1.99
1,2,4,5-Tetramethylbenzene	A	-1.29
Tetraphenylethylene	C	-2.05

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$
Aromatic	c hydrocarbons (continued)	
1,4,5,8-Tetraphenylnaphthalene	A	-1.39
Toluene	A	-1.98
1,2,3-Trimethylbenzene	A	-1.58
1,2,4-Trimethylbenzene	A	-1.41
1,3,5-Trimethylbenzene	A	-1.50
•	В	-1.90
Triphenylene	A	-1.46, -1.55
Triphenylmethane	C	-1.01, -1.68
•		-1.96
o-Xylene	A	-1.58, -2.04
<i>m</i> -Xylene	A	-1.58
<i>p</i> -Xylene	A	-1.56
	Aldehydes	
Acetaldehyde	B, pH 6.8–13	-1.89
Benzaldehyde	McIlvaine buffer, pH 2.2	-0.96, -1.32
Bromoacetaldehyde	pH 8.5	-0.40
	pH 9.8	-1.58, -1.82
Chloroacetaldehyde	Ammonia buffer, pH 8.4	-1.06, -1.66
Cinnamaldehyde	Buffer + EtOH, pH 6.0	-0.9, -1.5,
Crotonaldehyde	B, pH 1.3–2.0	-1.7 -0.92
,	Ammonia buffer, pH 8.0	-1.30
Dichloroacetaldehyde	Ammonia buffer, pH 8.4	-1.03, -1.67
3,7-Dimethyl-2,6-octadienal	0.1 M Et ₄ NI	-1.56, -2.22
Formaldehyde	$0.05 \mathrm{M}\mathrm{KOH} + 0.1 \mathrm{M}\mathrm{KCl}, \mathrm{pH}12.7$	-1.59
2-Furaldehyde	pH 1-8	-0.86,
3		−0.07 pH
	pH 10	-1.43
Glucose	Phosphate buffer, pH 7	-1.55
Glyceraldehyde	Britton–Robinson buffer, pH 5.0	-1.47
	Britton–Robinson buffer, pH 8.0	-1.55
Glycolaldehyde	0.1 M KOH, pH 13	-1.70
Glyoxal	B, pH 3.4	-1.41
4-Hydroxybenzaldehyde	Britton–Robinson buffer, pH 1.8	-1.16
	Britton–Robinson buffer, pH 6.8	-1.45
4-Hydroxy-2-methoxybenzaldehyde	McIlvaine buffer, pH 2.2	-1.05
J J J J J J J J J J J J J J J J J J J	McIlvaine buffer, pH 5.0	-1.16, -1.36
	McIlvaine buffer, pH 8.0	-1.47
o-Methoxybenzaldehyde	Britton–Robinson buffer, pH 1.8	-1.02
•	Britton–Robinson buffer, pH 6.8	-1.49
<i>p</i> -Methoxybenzaldehyde	Britton–Robinson buffer, pH 1.8	-1.17
. , , , , , , , , , , , , , , , , , , ,	Britton–Robinson buffer, pH 6.8	-1.48
Methyl glyoxal	A, pH 4.5	-0.83

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$	
	Aldehydes (continued)		
<i>m</i> -Nitrobenzaldehyde	Buffer + 10% EtOH, pH 2.0	-0.28, -1.20	
Phthalaldehyde	Buffer, pH 3.1	-0.64, -1.07	
•	Buffer, pH 7.3	-0.89, -1.29	
2-Propenal (acrolein)	pH 4.5	-1.36	
	pH 9.0	-1.1	
Propionaldehyde	0.1 M LiOH, pH 13	-1.93	
Pyrrole-2-carbaldehyde	0.1 M HCl + 50% EtOH	-1.25	
Salicylaldehyde	McIlvaine buffer, pH 2.2	-0.99, -1.23	
	McIlvaine buffer, pH 5.0	-1.20, -1.30	
	McIlvaine buffer, pH 8.0	-1.32	
Trichloroacetaldehyde	Ammonia buffer, pH 8.4	-1.35, -1.66	
·	0.1 M KCl + 50% EtOH	-1.55	
	Ketones		
Acetone	B, pH 9.3	-1.52	
	C	-2.46	
Acetophenone	D + McIlvaine buffer, pH 4.9	-1.33	
	D + McIlvaine buffer, pH 7.2	-1.58	
	D + McIlvaine buffer, pH 1.3	-1.08	
7H-Benz[de]anthracen-7-one			
Benzil	D + McIlvaine buffer, pH 1.3	-0.27	
	D + McIlvaine buffer, pH 4.9	-0.50	
Benzoin	D + McIlvaine buffer, pH 1.3	-0.90	
	D + McIlvaine buffer, pH 8.6	-1.49	
Benzophenone	D + McIlvaine buffer, pH 1.3	-0.94	
•	D + McIlvaine buffer, pH 8.6	-1.36	
Benzoylacetone	Buffer, pH 2.6	-1.60	
•	Buffer, pH 5.3 and pH 7.6	-1.68	
	Buffer, pH 9.7	-1.72	
Bromoacetone	0.1 M LiCl	-0.29	
2,3-Butanedione	0.1 M HCl	-0.84	
3-Buten-2-one	0.1 M KCl	-1.42	
Butyrophenone	0.1 M NH ₄ Cl + 50% EtOH	-1.55	
D-Carvone	$0.1 \mathrm{M} \mathrm{Et_4NI} + 80\% \mathrm{EtOH}$	-1.71	
Chloroacetone	0.1 M LiCl	-1.18	
Coumarin	McIlvaine buffer, pH 2.0	-0.95	
	McIlvaine buffer, pH 5.0	-1.11, -1.44	
Cyclohexanone	C	-2.45	
cis-Dibenzoylethylene	D, pH 1	-0.30	
	D, pH 11	-0.62, -1.65	
trans-Dibenzoylethylene	D, pH 1	-0.12	
	D, pH 11	-0.57, -1.52	
Dibenzoylmethane	D, pH 1.3	-0.59	
	D, pH 11.3	-1.30, -1.62	

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Solvent system	$E_{_{1/2}}$	
Ketones (continued)		
D, pH 2.0	-0.93	
A	-2.10	
D, pH 7.0	-0.6	
	-1.30	
+ 50% 2-PrOH, pH 6.1		
Acetate buffer + Me ₄ NOH	-1.51	
+ 50% 2-PrOH, pH 9.6		
Acetate buffer, pH 2.0	-0.50	
	-0.65	
Borate buffer, pH 10.1	-1.18, -1.44	
0.02 M LiCl	-1.76	
pH 8.2	-1.52	
1	-1.36	
	-1.46	
	-0.67, -0.83	
	-0.73, -1.01	
Britton–Robinson buffer, pH 6.8	-0.10, -0.90, -1.20	
Britton–Robinson buffer, pH 9.2	-1.35	
	-1.59, -2.08	
	1.65, 2.00	
	-0.3, -0.5	
	0.5, 0.5	
	-0.3, -0.5,	
, p	-0.8	
Phosphate buffer + citrate		
	-0.8	
	-0.64	
A	-1.28	
D + McIlvaine buffer, pH 1.3	-1.01	
D + McIlvaine buffer, pH 11.3	-1.60	
D, pH 1.3	-0.72	
D, pH 8.6	-1.27	
$0.1 \mathrm{M}\mathrm{Bu_4NI} + 50\%$ dioxane	-0.20	
pH 4.2	-1.1, -1.5	
pH 9.7	-1.2, -1.4	
Ĉ	-1.74	
Phosphate buffer $+ 1\%$ EtOH,	-0.56	
pH 8.0		
D + Britton–Robinson buffer,		
pH 2.6	-1.20	
p11 2.0		
D + Britton–Robinson buffer,		
1	-1.40	
D + Britton–Robinson buffer,	-1.40	
	Ketones (continued) D, pH 2.0 A D, pH 7.0 Acetate buffer + Me ₄ NOH + 50% 2-PrOH, pH 6.1 Acetate buffer + Me ₄ NOH + 50% 2-PrOH, pH 9.6 Acetate buffer, pH 2.0 Phthalate buffer, pH 5.0 Borate buffer, pH 10.1 0.02 M LiCl pH 8.2 D, pH 5 D, pH 5 Britton-Robinson buffer, pH 4.5 Britton-Robinson buffer, pH 6.8 Britton-Robinson buffer, pH 6.8 Britton-Robinson buffer + citrate buffer, pH 2.9 Phosphate buffer + citrate buffer, pH 4.3 Phosphate buffer + citrate buffer, pH 5.4 A A D + McIlvaine buffer, pH 1.3 D, pH 1.3 D, pH 1.3 D, pH 8.6 0.1 M Bu ₄ NI + 50% dioxane pH 4.2 pH 9.7 C Phosphate buffer + 1% EtOH, pH 8.0	

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$
	Quinones	
Anthraquinone	Acetate buffer + 40% dioxane, pH 5.6	-0.51
	Phosphate buffer + 40% dioxane, pH 7.9	-0.71
o-Benzoquinone	Britton–Robinson buffer, pH 7.0	+0.20
	Britton–Robinson buffer, pH 9.0	+0.08
2,3-Dimethylnaphthoquinone	D, pH 5.4	-0.22
1,2-Naphthoquinone	Phosphate buffer, pH 5.0	-0.03
	Phosphate buffer, pH 7.0	-0.13
1,4-Naphthoquinone	Britton–Robinson buffer, pH 7.0	-0.07
	Britton–Robinson buffer, pH 9.0	-0.19
	Acids	
Acetic acid	A	-2.3
Acrylic acid	pH 5.6	-0.85
Adenosine-5'-phosphoric acid	$HClO_4 + KClO_4$, pH 2.2	-1.13
4-Aminobenzenesulfonic acid	$0.05\mathrm{M}\mathrm{Me_4NI}$	-1.58
3-Aminobenzoic acid	pH 5.6	-0.67
Anthranilic acid	pH 5.6	-0.67
Ascorbic acid	Birtton–Robinson buffer, pH 3.4	+0.17
	Britton–Robinson buffer, pH 7.0	-0.06
Barbituric acid	Borate buffer, pH 9.3	-0.04
Benzoic acid	A	-2.1
Benzoylformic acid	Britton–Robinson buffer, pH 2.2	-0.48
•	Britton–Robinson buffer, pH 5.5	-0.85, -1.5
	Britton–Robinson buffer, pH 7.2	-0.98, -1.5
	Britton–Robinson buffer, pH 9.2	-1.25
Bromoacetic acid	pH 1.1	-0.54
2-Bromopropionic acid	pH 2.0	-0.39
Crotonic acid	C	-1.94
Dibromoacetic acid	pH 1.1	-0.03, -0.1
Dichloroacetic acid	pH 8.2	-1.57
5,5-Diethylbarbituric acid	Borate buffer, pH 9.3	0.00
Flavanol	D, pH 5.6	-1.25
	D, pH 7.7	-1.40
Folic acid	Britton–Robinson buffer, pH 4.6	-0.73
Formic acid	0.1 M KCl	-1.66
Fumaric acid	HCl + KCl, pH 2.6	-0.83
	Acetate buffer, pH 4.0	-0.93
	Acetate buffer, pH 5.9	-1.20
2,4-Hexadienedioic acid	Acetate buffer, pH 4.5	-0.97
Iodoacetic acid	pH 1	-0.16
Maleic acid	Britton–Robinson buffer, pH 2.0	-0.70
	Britton–Robinson buffer, pH 4.0	-0.97
	Britton–Robinson buffer, pH 6.0	-1.11, -1.

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Britton-Robinson buffer, pH 9.7 -1.51	$E_{1/2}$	
Methacrylic acid D+0.1 M LiCl -1.69 Nitrobenzoic acids Buffer + 10% EtOH, pH 2.0 -0.2, -0.2, -0.2, -0.2, -0.59 Oxalic acid B, pH 5.4-6.1 -1.80 2-Oxo-1,5-pentanedioic acid HCl + KCl, pH 1.8 -0.59 Ammonia buffer, pH 8.2 -1.30 2-Oxopropionic acid Britton-Robinson buffer, pH 5.6 -1.17 Britton-Robinson buffer, pH 9.7 -1.51 Phenolphthalein Phthalate buffer, pH 2.5 -0.67 Phthalate buffer, pH 4.7 -0.80 D, pH 9.6 -0.98 Picric acid pH 4.2 -0.34 pH 11.7 -0.36 -0.9 -0.9 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9 1,2-3-Trihydroxybenzoic acid Phosphate buffer, pH 8.8 +0.1 </td <td></td>		
Methacrylic acid D+0.1 M LiCl -1.69 Nitrobenzoic acids Buffer + 10% EtOH, pH 2.0 -0.2, -0.2, -0.2, -0.2, -0.59 Oxalic acid B, pH 5.4-6.1 -1.80 2-Oxo-1,5-pentanedioic acid HCl + KCl, pH 1.8 -0.59 Ammonia buffer, pH 8.2 -1.30 2-Oxopropionic acid Britton-Robinson buffer, pH 5.6 -1.17 Britton-Robinson buffer, pH 9.7 -1.51 Phenolphthalein Phthalate buffer, pH 2.5 -0.67 Phthalate buffer, pH 4.7 -0.80 D, pH 9.6 -0.98 Picric acid pH 4.2 -0.34 pH 11.7 -0.36 -0.9 -0.9 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9 1,2-3-Trihydroxybenzoic acid Phosphate buffer, pH 8.8 +0.1 </td <td></td>		
Nitroberzoic acids Buffer + 10% EtOH, pH 2.0 -0.2, -1.80 Oxalic acid B, pH 5.4–6.1 -1.80 2-Oxo-1,5-pentanedioic acid HCI+KCl, pH 1.8 -0.59 Ammonia buffer, pH 8.2 -1.30 2-Oxopropionic acid Britton-Robinson buffer, pH 5.6 -1.17 Britton-Robinson buffer, pH 9.7 -1.51 Phenolphthalein Phthalate buffer, pH 2.5 -0.67 Phthalate buffer, pH 4.7 -0.80 D, pH 9.6 -0.98 pH 4.2 -0.34 pH 11.7 -0.36 -0.9 -0.9 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid pH 7.0 -2.1 1,2,3-Propenetricarboxylic acid pH 5.0 -0.84 Phosphate buffer, pH 8.2 -0.84 Phosphate buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9 3,4,5-Trihydroxybenzoic acid Phosphate buffer, pH 8.8 +0.1 p-Aminophenol Britton-Robinson buffer, pH 8.6 +0.50 Britton-Robinson buffer, pH 8.6 Britton-Robinson		
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Ammonia buffer, pH 8.2 2-Oxopropionic acid Britton–Robinson buffer, pH 5.6 Britton–Robinson buffer, pH 6.8 Britton–Robinson buffer, pH 9.7 Phenolphthalein Phenolphthalein Phihalate buffer, pH 2.5 Phihalate buffer, pH 4.7 D, pH 9.6 Picric acid PH 4.2 Phosphate buffer, pH 8.2 Phosphate buffer, pH 10.4 Phosphate buffer, pH 10.4 Phosphate buffer, pH 10.4 Phosphate buffer, pH 8.8 P-Aminophenol P-Aminophenol Britton–Robinson buffer, pH 8.8 Britton–Robinson buffer, pH 8.8 Britton–Robinson buffer, pH 10.4 Britton–Robinson buffer, pH 8.6 Britton–Robinson buffer, pH 12.0 Phosphate buffer, pH 12.0 Phosphate buffer, pH 12.0 Phosphate buffer, pH 12.0 Phosphate buffer, pH 5.6 Britton–Robinson buffer, pH 12.0 Phosphate buffer, pH 12.0 Phosphate buffer, pH 5.6 Britton–Robinson buffer, pH 5.6 P-Cresol Ph 5.6 P-Cr		
Britton-Robinson buffer, pH 5.6 Britton-Robinson buffer, pH 6.8 Britton-Robinson buffer, pH 6.8 Britton-Robinson buffer, pH 9.7 -1.51		
Britton-Robinson buffer, pH 6.8 Britton-Robinson buffer, pH 9.7 -1.51		
Britton-Robinson buffer, pH 9.7 -1.51		
Phenolphthalein Phthalate buffer, pH 2.5 -0.67 Phthalate buffer, pH 4.7 -0.80 D, pH 9.6 -0.98 pH 4.2 -0.34 pH 11.7 -0.36 1,2,3-Propenetricarboxylic acid pH 7.0 Trichloroacetic acid Ammonia buffer, pH 8.2 Phosphate buffer, pH 10.4 -0.84 Phosphate buffer, pH 10.4 -0.94 3,4,5-Trihydroxybenzoic acid Phosphate buffer, pH 8.8 +0.1 p-Aminophenol Britton-Robinson buffer, pH 8.8 +0.1 p-Aminophenol Britton-Robinson buffer, pH 8.6 -0.04 Britton-Robinson buffer, pH 8.6 -0.04 Britton-Robinson buffer, pH 12.0 -0.16 o-Chlorophenol pH 5.6 -0.63 m-Chlorophenol pH 5.6 -0.65 o-Cresol pH 5.6 -0.65 p-Cresol pH 5.6 -0.56 n-Cresol pH 5.6 -0.35 1,3-Dihydroxybenzene pH 5.6 -0.61 1,4-Dihydroxybenzene pH 5.6 -0.23 o-Methoxyphenol	-1.53	
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Picric acid pH 4.2 -0.34 pH 11.7 -0.36 1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, -0.9, 3,4,5-Trihydroxybenzoic acid Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 8.8 +0.1 Phosphate buffer, pH 8.6 -0.04 Britton-Robinson buffer, pH 8.6 -0.046	-1.35	
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1,2,3-Propenetricarboxylic acid pH 7.0 -2.1 Trichloroacetic acid Ammonia buffer, pH 8.2 -0.84 Phosphate buffer, pH 10.4 -0.9, 3,4,5-Trihydroxybenzoic acid Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 8.8 +0.1 Phosphate buffer, pH 9.9 +0.50 Phosphate buffer, pH 9.8 +0.1 Phosphate buffer, pH 9.6 -0.04 Britton-Robinson buffer, pH 6.3 -0.04 Ph 5.6 -0.65 Ph 5.6 -0.65 Ph 5.6 -0.54 1,2-Dihydroxybenzene <	-0.56,	
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Phosphate buffer, pH 10.4 -0.9 -0.50 Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 8.8 +0.1 Phosphate buffer, pH 8.9 +0.50 Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 9.9 +0.50 Phosphate buffer, pH 10.4 +0.50 Phosphate buffer, pH 10.9 +0.50 Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 2.9 +0.50 Phosphate buffer, pH 6.3 +0.14 Phosphate buffer, pH 10.9 Phosphate buffer, pH 6.3 +0.14 Phosphate buffer, pH 10.4 Phosphate buffer, pH 10.4 Phosphate buffer, pH 6.3 Phosphate buffer, pH 6.6 +0.14 Phosphate buffer,	-1.57	
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o-Cresol pH 5.6 -0.56 m -Cresol pH 5.6 -0.61 p -Cresol pH 5.6 -0.54 1,2-Dihydroxybenzene pH 5.6 -0.35 1,3-Dihydroxybenzene pH 5.6 -0.61 1,4-Dihydroxybenzene pH 5.6 -0.23 o -Methoxyphenol pH 5.6 -0.46 m -Methoxyphenol pH 5.6 -0.62 p -Methoxyphenol pH 5.6 -0.41		
m-Cresol pH 5.6 -0.61 p -Cresol pH 5.6 -0.54 1,2-Dihydroxybenzene pH 5.6 -0.35 1,3-Dihydroxybenzene pH 5.6 -0.61 1,4-Dihydroxybenzene pH 5.6 -0.23 o -Methoxyphenol pH 5.6 -0.46 m -Methoxyphenol pH 5.6 -0.62 p -Methoxyphenol pH 5.6 -0.62 p -Methoxyphenol pH 5.6 -0.41		
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1,3-Dihydroxybenzene pH 5.6 -0.61 1,4-Dihydroxybenzene pH 5.6 -0.23 o-Methoxyphenol pH 5.6 -0.46 m-Methoxyphenol pH 5.6 -0.62 p-Methoxyphenol pH 5.6 -0.41		
o-MethoxyphenolpH 5.6 -0.46 m -MethoxyphenolpH 5.6 -0.62 p -MethoxyphenolpH 5.6 -0.41		
m-MethoxyphenolpH 5.6 -0.62 p -MethoxyphenolpH 5.6 -0.41		
<i>p</i> -Methoxyphenol pH 5.6 -0.41		
1-Naphthol A -0.74		
2-Naphthol A -0.82		
1,2,3-Trihydroxybenzene Britton–Robinson buffer, pH 3.1 +0.35		
Britton–Robinson buffer, pH 6.5 +0.10		
Britton–Robinson buffer, pH 9.5 -0.10		
Halogen compounds		
Bromobenzene A -1.98		
C 1.76		
1-Bromobutane C 2.32 1-Bromobutane C -2.27		
1 Diomoduline C 2.21		

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$		
Halogen compounds (continued)				
Bromoethane	С	-2.08		
Bromomethane	C	-1.63		
1-Bromonaphthalene (also		1.03		
2-bromonaphthalene)	A	-1.55, -1.60		
3-Bromo-1-propene	C	-1.29		
p-Bromotoluene	A	-1.72		
Carbon tetrachloride	C	-0.78, -1.71		
Chlorobenzene	A	-2.07		
Chloroform	C	-1.63		
Chloromethane	C	-2.23		
3-Chloro-1-propene	C	-1.91		
α -Chlorotoluene	C	-1.81		
p-Chlorotoluene	A	-1.76		
N-Chloro-p-toluenesulfonamide	0.5 M K ₂ SO ₄	-0.13		
9,10-Dibromoanthracene	A	-1.15, -1.47		
p-Dibromobenzene	C	-2.10		
1.2-Dibromobutane	$D + 1\% Na_2SO_3$	-1.45		
Dibromoethane	C C	-1.48		
meso-2,3-Dibromosuccinic acid	Acetate buffer, pH 4.0	-0.23, -0.89		
Dichlorobenzenes	C	-2.5		
Dichloromethane	C	-1.60		
Diiodomethane	C	-1.12, -1.53		
Hexabromobenzene	C	-0.8, -1.5		
Hexachlorobenzene	C	-1.4, -1.7		
Iodobenzene	A	-1.72		
Iodoethane	С	-1.67		
Iodomethane	A	-2.12		
	С	-1.63		
Tetrabromomethane	С	-0.3, -0.75,		
		-1.49		
Tetraiodomethane	С	-0.45, -1.05,		
		-1.46		
Tribromomethane	C	-0.64, -1.47		
α, α, α -Trichlorotoluene	C	-0.68, -1.65,		
		-2.00		
Nitro	and nitroso compounds	1		
1,2-Dinitrobenzene	Phthalate buffer, pH 2.5	-0.12, -0.32, -1.26		
	Borate buffer, pH 9.2	-0.38, -0.74		
1,3-Dinitrobenzene	Phthalate buffer, pH 2.5	-0.17, -0.29		
1,5 Dimitouenzene	Borate buffer, pH 9.2	-0.46, -0.68		
1,4-Dinitrobenzene	Phthalate buffer, pH 2.5	-0.40, -0.08 -0.12, -0.33		
1,7 Dilliuoodizene	Borate buffer, pH 9.2	-0.12, -0.35 -0.35, -0.80		
	Borate buffer, pri 3.2	0.55, 0.60		

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$	
Nitro and nitroso compounds (continued)			
Methyl nitrobenzoates	Buffer + 10% EtOH, pH 2.0	-0.20 to -0.25 -0.68 to -0.74	
p-Nitroacetophenone	Britton–Robinson buffer, pH 2.2	-0.16, -0.61, -1.09	
	Britton–Robinson buffer, pH 10.0	-0.51, -1.40, -1.73	
o-Nitroaniline	0.03 M LiCl + 0.02 M benzoic acid in EtOH	-0.88	
<i>m</i> -Nitroaniline	Britton–Robinson buffer, pH 4.3 Briton-Robinson buffer, pH 7.2 Britton–Robinson buffer, pH 9.2	-0.3, -0.8 -0.5 -0.7	
<i>p</i> -Nitroaniline	pH 2.0 Acetate buffer, pH 4.6	-0.36 -0.5	
o-Nitroanisole	Buffer + 10% EtOH, pH 2.0	-0.29, -0.58	
<i>p</i> -Nitroanisole	Buffer + 10% EtOH, pH 2.0	-0.35, -0.64	
1-Nitroanthraquinone	Britton–Robinson buffer, pH 7.0	-0.16	
Nitrobenzene	HCl + KCl + 8% EtOH, pH 0.5	-0.16, -0.76	
	Phthalate buffer, pH 2.5	-0.30	
	Borate buffer, pH 9.2	-0.70	
Nitrocresols	Britton–Robinson buffer, pH 2.2	-0.2 to -0.3	
	Britton–Robinson buffer, pH 4.5	-0.4 to -0.5	
Nitroethane	Britton–Robinson buffer, pH 8.0 Britton–Robinson buffer + 30% MeOH, pH 1.8	-0.6 -0.7	
	Britton–Robinson buffer + 30% MeOH, pH 4.6	-0.8	
2-Nitrohydroquinone	Phosphate buffer + citrate buffer, pH 2.1	-0.2	
	Phosphate buffer + citrate buffer, pH 5.2	-0.4	
	Phosphate buffer + citrate buffer, pH 8.0	-0.5	
Nitromethane	Britton–Robinson buffer + 30% MeOH, pH 1.8	-0.8	
	Britton–Robinson buffer + 30% MeOH, pH 4.6	-0.85	
o-Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	-0.23	
	Britton–Robinson buffer + 10% EtOH, pH 4.0	-0.4	
	Britton–Robinson buffer + 10% EtOH, pH 8.0	-0.65	
	Britton–Robinson buffer + 10% EtOH, pH 10.0	-0.80	

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system	$E_{1/2}$
Nitro and n	itroso compounds (continued)	•
m-Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	-0.37
	Britton–Robinson buffer + 10% EtOH, pH 4.0	-0.40
	Britton–Robinson buffer + 10% EtOH, pH 8.0	-0.64
	Britton–Robinson buffer + 10% EtOH, pH 10.0	-0.76
<i>p</i> -Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	-0.35
	Britton–Robinson buffer + 10% EtOH, pH 4.0	-0.50
	Britton–Robinson buffer + 10% EtOH, pH 8.0	-0.82
1-Nitropropane	Britton–Robinson buffer + 30% MeOH, pH 1.8	-0.73
	Britton–Robinson buffer + 30% MeOH, pH 8.6	-0.88
	Britton–Robinson buffer + 30% MeOH, pH 8.0	-0.95
2-Nitropropane	McIlvaine buffer, pH 2.1 McIlvaine buffer, pH 5.1	-0.53 -0.81
Nitrosobenzene	McIlvaine buffer, pH 6.0 McIlvaine buffer, pH 8.0	-0.03 -0.14
1-Nitroso-2-naphthol	D + buffer, pH 4.0 D + buffer, pH 7.0 D + buffer, pH 9.0	+0.02 -0.20 -0.31
<i>N</i> -Nitrosophenylhydroxylamine <i>o</i> -Nitrotoluene	pH 2.0 Phthalate buffer, pH 2.5	$ \begin{array}{c c} -0.84 \\ -0.35, -0.66 \end{array} $
<i>m</i> -Nitrotoluene (also <i>p</i> -nitrotoluene)	Phthalate buffer, pH 7.4 Phthalate buffer, pH 2.5	-0.60, -1.06 -0.30, -0.53
Tetranitromethane 1,3,5-Trinitrobenzene	Phthalate buffer, pH 7.4 pH 12.0 Phthalate buffer, pH 4.1	-0.58, -1.06 -0.41 -0.20, -0.29,
	Borate buffer, pH 9.2	$ \begin{array}{r} -0.34 \\ -0.34, -0.48, \\ -0.65 \end{array} $
Heterocyclic	compounds containing nitrogen	
Acridine	D, pH 8.3	-0.80, -1.45
Cinchonine	B, pH 3	-0.90
2-Furanmethanol	Britton Pobinson buffer, pH 2.0	-0.96 -1.38 -1.70
2-Hydroxyphenazine	Britton–Robinson buffer, pH 5.8 Britton–Robinson buffer, pH 4.0	-1.38, -1.70 -0.24

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TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound Solvent system		$E_{1/2}$		
Heterocyclic compounds containing nitrogen (continued)				
8-Hydroxyquinoline	B, pH 5.0	-1.12		
	Phosphate buffer, pH 8.0	-1.18, -1.71		
3-Methylpyridine	D + 0.1 M LiCl	-1.76		
4-Methylpyridine	D + 0.1 M LiCl	-1.87		
Phenazine	Phosphate buffer + citrate buffer, -0.36 pH 7.0 Phosphate buffer + citrate buffer, -1.75			
Pyridine	Phosphate buffer + citrate buffer, pH 7.0	-1.75		
Pyridine-2-carboxylic acid	B, pH 4.1	-1.10		
, , , , , , , , , , , , , , , , , , ,	B, pH 9.3	-1.48, -1.94		
Pyridine-3-carboxylic acid	0.1 M HCl	-1.08		
Pyridine-4-carboxylic acid	Britton–Robinson buffer, pH 6.1	-1.14		
·	pH 9.0	-1.39, -1.68		
Pyrimidine	Citrate buffer, pH 3.6	-0.92, -1.24		
•	Ammonia buffer, pH 9.2	-1.54		
Quinoline-8-carboxylic acid	pH 9	-1.11		
Quinoxaline	Phosphate buffer + citrate buffer, pH 7.0	-0.66, -1.52		
Azo, hydrazine	hydroxylamine, and oxime compounds			
Azobenzene	D, pH 4.0	-0.20		
	D, pH 7.0	-0.50		
Azoxybenzene	Buffer + 20% EtOH, pH 6.3	-0.30		
Benzoin-1-oxime	Buffer, pH 2.0	-0.88		
	Buffer, pH 5.6	-1.08		
	Buffer, pH 8.2	-1.67		
Benzoylhydrazine	0.13 M NaOH, pH 13.0	-0.30		
Dimethylglyoxime	Ammonia buffer, pH 9.6	-1.63		
Hydrazine	Britton–Robinson buffer, pH 9.3	-0.09		
Hydroxylamine	Britton–Robinson buffer, pH 4.6	-1.42		
	Britton–Robinson buffer, pH 9.2 –1.65			
Oxamide	Acetate buffer -1.55			
Phenylhydrazine	McIlvaine buffer, pH 2	+0.19		
	0.13 M NaOH, pH 13.0	-0.36		
Phenylhydroxylamine	McIlvaine buffer + 10% EtOH, pH 2	-0.68		
2 1001,9 11.9 (2001.) 141111110	McIlvaine buffer + 10% EtOH,	-0.33		
	McIlvaine buffer + 10% EtOH, pH 4–10	-0.33 0.061 pH		
Salicylaldoxime	McIlvaine buffer + 10% EtOH, pH 4–10 Phosphate buffer, pH 5.4	1		
	McIlvaine buffer + 10% EtOH, pH 4–10	0.061 pH		

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at $25\,^{\circ}\text{C}$ (continued)

Compound	Solvent system $E_{1/2}$			
	Indicators and dyestuffs			
Brilliant Green $HCl + KCl$, pH 2.0 -0.2 , -0				
Indigo carmine	pH 2.5	-0.24		
Indigo disulfonate	pH 7.0	-0.37		
Malachite Green G	HCl + KCl, pH 2.0	-0.2, -0.5		
Metanil yellow	Phosphate buffer + 1% EtOH, pH 7.0	-0.51		
Methylene blue	Britton–Robinson buffer, pH 4.9	-0.15		
•	Britton–Robinson buffer, pH 9.2	-0.30		
Methylene green	Phosphate buffer + 1% EtOH, pH 7.0	-0.12		
Methyl orange	Phosphate buffer + 1% EtOH, pH 7.0	-0.51		
Morin	D, pH 7.6	-1.7		
Neutral red	Britton–Robinson buffer, pH 2.0	-0.21		
	Britton–Robinson buffer, pH 7.0	-0.57		
	Peroxide			
Ethyl peroxide	Ethyl peroxide 0.02 M HCl -0.2			

SECTION 9

DATA USEFUL IN LABORATORY MANIPULATION AND ANALYSIS

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9.2 SECTION 9

COOLING MIXTURES

Convenient cooling mixtures can be prepared in several ways. First, an inorganic salt may be mixed with finely shaved dry ice. Such a mixture can be used to maintain temperatures as shown in Table 9.1.

TABLE 9.1 Cooling Mixtures Made from Dry Ice and Salts

Salt	Dry ice, g/100 g	Minimum temperature, °C
CaCl ₂ ·6H ₂ O	41 81 123 143	-9.0 -21.5 -40.3 -55
NH ₄ Cl NaBr MgCl ₂	25 66 85	-15.4 -28 -34

A more common method for preparing a low temperature bath is to mix an organic substance with either dry ice or liquid nitrogen. Dry ice $(CO_2, -78^{\circ}C)$ can be added in small lumps to the solvent until a slight excess of dry ice remains. Alternately, liquid nitrogen $(N_2, -196^{\circ}C)$ can be poured into the solvent until a slush is formed that consists of the solid–liquid mixture at its melting point.

TABLE 9.2 Dry Ice or Liquid Nitrogen Slush Baths

Substance	Temperature, °C	Substance	Temperature, °C
Ethylene glycol 1,2-Dichlorobenzene Carbon tetrachloride Bromobenzene Methoxybenzene Chlorobenzene Bis(2-ethoxyethyl) ether N-Methylaniline p-Cymene	-13 -17 -22.9 -31 -37 -45 -44 -57 -68	Acetone–CO ₂ Ethyl acetate 2-Butanone Hexane Methanol Carbon disulfide Bromoethane Pentane 2-Methylbutane	-77 -84 -87 -95 -98 -112 -119 -130 -160

HUMIDIFICATION AND DRYING

A saturated aqueous solution in contact with an excess of a definite solid phase at a given temperature will maintain constant humidity in an enclosed space. Table 9.3 identifies a number of salts suitable for this purpose. The aqueous tension (in millimeters of Hg) of a solution at a given temperature is found by multiplying the decimal fraction of the humidity by the aqueous tension at 100% humidity for the specific temperature. For example, the aqueous tension of a saturated solution of NaCl at 20° C is $0.757 \times 17.54 = 13.28$ mmHg and at 80° C is $0.764 \times 355.1 = 271.3$ mmHg.

TABLE 9.3 Humidity (%) Maintained by Saturated Solutions of Various Salts at Specified Temperatures

Solid phase	Temperature, °C							
	10	20	25	30	40	60	80	
K ₂ Cr ₂ O ₇			98.0					
K_2SO_4	98	97	97	96	96	96		
KNO ₃	95	93	92.5	91	88	82		
KCl	88	85.0	84.3	84	81.7	80.7	79.5	
KBr	86	84	80.7		79.6	79.0	79.3	
NaCl	76	75.7	75.3	74.9	74.7	74.9	76.4	
NaNO ₃	77	75	73.8	72.8	71.5	67.5	65.5	
KI					66.8	63.1	60.8	
NaNO ₂		66	65	63.0	61.5	59.3	58.9	
Na ₂ CrO ₄ ·4H ₂ O				64.6	61.8	55.6	56.2	
$NaBr \cdot 2H_2O$	58	57.9	57.7		52.4	49.9	50.0	
$Na_2Cr_2O_7 \cdot 2H_2O$	58	55	54		53.6	55.2	56.0	
$Mg(NO_3)_2 \cdot 6H_2O$	57	55	52.9	52	49	43		
$K_2CO_3 \cdot 2H_2O$	47	44	42.8	42	40			
$NaI \cdot 2H_2O$		47		36.4	32.3	25.3	23.2	
$MgCI_2 \cdot 6H_2O$	34	33	33.0	33	32	30		
CaCl ₂ ·6H ₂ O	38	32.6	29	26				
$KF \cdot 2H_2O$				27.4	22.8	21.0	22.8	
$KC_2H_3O_2 \cdot 1.5H_2O$	24	23	22.5	22	20			
LiCl·H ₂ O	13	12	11.1	12	11	11		
KOH	13	9	8	7	6	5		
Aqueous tension at 100%								
humidity, mmHg	9.21	17.54	23.76	31.82	55.32	149.4	355.1	

TABLE 9.4 Humidity (%) Maintained by Saturated Solutions of Common Salts at Specified Temperatures

Solid phase	Temperature, °C	Humidity, %		
KF	100	22.9		
KI	100	56.2		
$(NH_4)_2SO_4$	20–30	81.1		
	108	75		
BaCl ₂ ·2H ₂ O	25	90.2		
NaF	100	96.6		

Drying agent

Al_2O_3	Hydrocarbons	0.002-0.005	0.2	175 (24 h)
$Ba(ClO_4)_2^a$	Inert gas streams	0.6-0.8	0.17	140
BaO	Basic gases: hydrocarbons, aldehydes, alcohols	0.0007-0.003	0.12	1000
CaC ₂ ^b	Ethers		0.56	Impossible
CaCl ₂ ^c	Inert organics	0.1–0.2	0.15 (1 H ₂ O) 0.30 (2 H ₂ O)	250
CaH ₂ ^d	Hydrocarbons, ethers, amines, esters, higher alcohols	1×10^{-5}	0.85	Impossible
CaO	Ethers, esters, alcohols, amines	0.01-0.003	0.31	Difficult, 1000
CaSO ₄	Most organic substances	0.005-0.07	0.07	225
Dow Desiccant 812e	Most materials	(5–200 ppm)		No
K ₂ CO ₃	Most materials except acids and phenols		0.16	158
KOH	Amines	0.01-0.9		Impossible
LiAlH ₄ ^f	Hydrocarbons		1.9	Impossible
$Mg(ClO_4)_2^a$	Gas streams	0.0005-0.002	0.24	250 (high vacuum)
MgO	All but acidic compounds	0.008	0.45	800
MgSO ₄	Most organic compounds	1–12	0.15-0.75	Not feasible
Molecular sieves				
4X	Molecules with effective diameter > 4Å	0.001	0.18	250
5X	Molecules with effective diameter > 5Å	0.001	0.18	250
9.5% Na–Pb alloy ^d	Hydrocarbons, ethers	(For solvents only)	0.08	Impossible
Na ₂ SO ₄	Ketones, acids, alkyl and aryl halides	12	1.25	150
P_2O_5	Gas streams; not suitable for alcohols, amines, ketones, or amines	2×10^{-5}	0.5	Not feasible
Silica gel	Most organic amines	0.002-0.07	0.2	200-350
Sulfuric acid	Air and inert gas streams	0.003-0.008	Indefinite	Not feasible

Most useful for

Residual water, mg H₂O

per liter of dry air (25°C)

Regeneration,

°C

Grams water removed

per gram of desiccant

bExplosive C₂H₂ formed. Drying action slow. dH₂ formed.

^eUsed for column drying of organic liquids.

^fStrong reductant.

SEPARATION METHODS

TABLE 9.6 Solvents of Chromatographic Interest (arranged in order of increasing solvent strength)

Solvent	Boiling point,	Solvent streng	Solvent strength parameter		Refractive index	UV
	°C	e° (SiO ₂)	e° (Al ₂ O ₃)	$\begin{array}{c} \text{mN} \cdot \text{s} \cdot \text{m}^{-2} \\ (20^{\circ}\text{C}) \end{array}$	(20°C)	cutoff, nm
Fluoroalkanes			-0.25		1.25	
Pentane	36	0.0	0.0	0.24 ^{15 ℃}	1.358	210
Hexane	69	0.0	0.0	0.31	1.375	210
2,2,4-Trimethylpentane	99		0.01	0.50	1.392	215
Decane	174		0.04	0.93	1.412	210
Cyclohexane	81	-0.05	0.04	0.98	1.426	210
Cyclopentane	49		0.05	0.44	1.407	210
Diisobutylene	101		0.06		1.411	
1-Pentene	30		0.08	0.24°°C	1.371	
Carbon disulfide	46	0.14	0.15	0.36	1.626	380
Carbon tetrachloride	77	0.14	0.18	0.97	1.466	265
1-Chlorobutane	78		0.26	0.43	1.402	220
1-Chloropentane	98		0.26	0.58	1.412	225
o-Xylene	144		0.26	0.81	1.505	290
Diisopropyl ether	68		0.28	0.38 ²⁵ °C	1.369	220
2-Chloropropane	35		0.29	0.33	1.378	225
Toluene	111		0.29	0.59	1.497	286
1-Chloropropane	47		0.30	0.35	1.389	225
Chlorobenezene	132		0.40	0.80	1.525	
Benzene	80	0.25	0.32	0.65	1.501	280
Bromoethane	38		0.37	0.40	1.424	
Diethyl ether	35	0.38	0.38	0.25	1.353	218
Diethyl sulfide	92		0.38	0.45	1.443	290
Chloroform	62	0.26	0 40	0.57	1.443	245

TABLE 9.6 Solvents of Chromatographic Interest (continued)

	Boiling Solvent stre		ngth parameter	Viscosity, mN·s·m ⁻²	Refractive index	UV
Solvent	°C	e° (SiO ₂)	<i>e</i> ° (Al ₂ O ₃)	(20°C)	(20°C)	cutoff, nm
Dichloromethane	41		0.42	0.44	1.425	235
4-Methyl-2-pentanone	116		0.43	0.42 ^{15 °C}	1.396	335
Tetrahydrofuran	66		0.45	0.55	1.407	220
1,2-Dichloroethane	84		0.49	0.80	1.445	228
2-Butanone	80		0.51	0.42 ^{15 °C}	1.379	330
1-Nitropropane	131		0.53	0.80 ^{25°C}	1.402	380
Acetone	56	0.47	0.56	0.32	1.359	330
1,4-Dioxane	101	0.49	0.56	1.44 ¹⁵ °C	1.420	215
Ethyl acetate	77	0.38	0.58	0.45	1.372	255
Methyl acetate	56		0.60	0.48 ¹⁵ °C	1.362	260
1-Pentanol	138		0.61	4.1	1.410	210
Dimethyl sulfoxide	189		0.62	2.47	1.478	265
Aniline	184		0.62	4.40	1.586	
Diethylamine	56		0.63	0.33	1.386	275
Nitromethane	101		0.64	0.67	1.394	380
Acetonitrile	82	0.50	0.65	0.37	1.344	190
Pyridine	115		0.71	0.97	1.510	330
2-Butoxyethanol	170		0.74	3.15 ^{25°C}	1.420	220
1-Propanol	97		0.82	2.25	1.386	210
2-Propanol	82		0.82	2.50	1.377	210
Ethanol	78		0.88	1.20	1.361	210
Methanol	65		0.95	0.59	1.328	210
Ethylene glycol	198		1.11	21.8	1.432	210
Acetic acid	118		large	1.23	1.372	260
Water	100		large	1.00	1.333	191

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25 °C

		ı			
		Refrac	tive		
		inde		Density,	g/mL
				•	
Solvent 1	Solvent 2	1	2	1	2
Acetone	Ethanol	1.357	1.359	0.788	0.786
Ethyl formate	Methyl acetate	1.358	1.360	0.766	0.786
Ethanol	Propionitrile	1.359	1.363	0.786	0.777
2,2-Dimethylbutane	2-Methylpentane	1.366	1.369	0.760	0.649
2-Methylpentane	Hexane	1.369	1.372	0.649	0.655
Isopropyl acetate	2-Chloropropane	1.375	1.376	0.868	0.865
3-Butanone	Butyraldehyde	1.377	1.378	0.801	0.803
Butyraldehyde	Butyronitrile	1.377	1.382	0.799	0.786
Dipropyl ether	Butyl ethyl ether	1.379	1.382	0.753	0.746
		1.379	1.382	0.733	0.740
Propyl acetate	Ethyl propionate				
Propyl acetate	1-Chloropropane	1.382	1.386	0.883	0.890
Butyronitrile	2-Methyl-2-propanol	1.382	1.385	0.786	0.781
Ethyl propionate	1-Chloropropane	1.382	1.386	0.888	0.890
1-Propanol	2-Pentanone	1.383	1.387	0.806	0.804
Isobutyl formate	1-Chloropropane	1.383	1.386	0.881	0.890
1-Chloropropane	Butyl formate	1.386	1.387	0.890	0.888
Butyl formate	Methyl butyrate	1.387	1.391	0.888	0.875
Methyl butyrate	2-Chlorobutane	1.392	1.395	0.875	0.868
Butyl acetate	2-Chlorobutane	1.392	1.395	0.877	0.868
4-Methyl-2-pentanone	Pentanonitrile	1.394	1.395	0.797	0.795
4-Methyl-2-pentanone	1-Butanol	1.394	1.397	0.797	0.812
2-Methyl-1-propanol	Pentanonitrile	1.394	1.395	0.798	0.795
2-Methyl-1-propanol	2-Hexanone	1.394	1.395	0.798	0.810
2-Butanol	2,4-Dimethyl-3-pentanone	1.395	1.399	0.803	0.805
2-Hexanone	1-Butanol	1.395	1.397	0.810	0.812
Pentanonitrile	2,4-Dimethyl-3-pentanone	1.395	1.399	0.795	0.805
2-Chlorobutane	Isobutyl butyrate	1.395	1.399	0.868	0.860
Butyric acid	2-Methoxyethanol	1.396	1.400	0.955	0.960
1-Butanol	3-Methyl-2-pentanone	1.397	1.398	0.812	0.808
1-Chloro-					
2-methylpropane	Isobutyl butyrate	1.397	1.399	0.872	0.860
1-Chloro-					
2-methylpropane	Pentyl acetate	1.397	1.400	0.872	0.871
Methyl methacrylate	3-Methyl-2-pentanone	1.398	1.398	0.795	0.808
Triethylamine	2,2,3-Trimethylpentane	1.399	1.401	0.723	0.712
Butylamine	Dodecane	1.399	1.400	0.736	0.746
Isobutyl butyrate	1-Chlorobutane	1.399	1.401	0.860	0.875
1-Nitropropane	Propionic anhydride	1.399	1.400	0.995	1.007
Pentyl acetate	1-Chlorobutane	1.400	1.400	0.871	0.881
Pentyl acetate	Tetrahydrofuran	1.400	1.404	0.871	0.885
Dodecane	Dipropylamine	1.400	1.400	0.746	0.736
1-Chlorobutane	Tetrahydrofuran	1.401	1.404	0.871	0.885
Isopentanoic acid	2-Ethoxyethanol	1.402	1.405	0.923	0.926
Dipropylamine	Cyclopentane	1.402	1.403	0.736	0.740
2-Pentanol	4-Heptanone	1.403	1.404	0.730	0.740
3-Methyl-1-butanol	Hexanonitrile	1.404	1.405	0.804	0.813
	4-Heptanone	1.404			
3-Methyl-1-butanol Hexanonitrile	4-Heptanone 4-Heptanone	1.404	1.405 1.405	0.805 0.801	0.813 0.813
TICAMOINUNE	4-11eptanone	1.403	1.403	0.001	0.013

9.8 SECTION 9

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25 °C (*continued*)

		Refra		Density,	g/mL
Solvent 1	Solvent 2	1	2	1	2
Hexanonitrile	1-Pentanol	1.405	1.408	0.801	0.810
Hexanonitrile	2-Methyl-1-butanol	1.405	1.409	0.801	0.815
4-Heptanone	1-Pentanol	1.405	1.408	0.813	0.810
2-Ethoxyethanol	Pentanoic acid	1.405	1.406	0.926	0.936
2-Heptanone	1-Pentanol	1.406	1.408	0.811	0.810
2-Heptanone	2-Methyl-1-butanol	1.406	1.409	0.811	0.815
2-Heptanone	Dipentyl ether	1.406	1.410	0.811	0.799
2-Pentanol	3-Isopropyl-2-pentanone	1.407	1.409	0.804	0.808
1-Pentanol	Dipentyl ether	1.408	1.410	0.810	0.799
2-Methyl-1-butanol	Dipentyl ether	1.409	1.410	0.815	0.799
Isopentyl isopentanoate	Allyl alcohol	1.410	1.411	0.853	0.847
Dipentyl ether	2-Octanone	1.410	1.414	0.799	0.814
2,4-Dimethyldioxane	3-Chloropentene	1.412	1.413	0.935	0.932
2,4-Dimethyldioxane	Hexanoic acid	1.412	1.415	0.935	0.923
Diethyl malonate	Ethyl cyanoacetate	1.412	1.415	1.051	1.056
3-Chloropentene	Octanoic acid	1.413	1.415	0.932	0.923
2-Octanone	1-Hexanol	1.414	1.416	0.814	0.814
2-Octanone	Octanonitrile	1.414	1.418	0.814	0.810
3-Octanone	3-Methyl-2-heptanone	1.414	1.416	0.830	0.818
3-Methyl-2-heptanone	1-Hexanol	1.415	1.416	0.818	0.814
3-Methyl-2-heptanone	Octanonitrile	1.415	1.418	0.818	0.810
1-Hexanol	Octanonitrile	1.416	1.418	0.814	0.810
Dibutylamine	Allylamine	1.416	1.419	0.756	0.758
Allylamine	Methylcyclohexane	1.419	1.421	0.758	0.765
Butyrolactone	1,3-Propanediol	1.434	1.438	1.051	1.049
Butyrolactone	Diethyl maleate	1.434	1.438	1.051	1.064
2-Chloromethyl-2- propanol	Diethyl maleate	1.436	1.438	1.059	1.064
N-Methylmorpholine	Dibutyl decanedioate	1.436	1.440	0.924	0.932
1,3-Propanediol	Diethyl maleate	1.438	1.438	1.049	1.064
Methyl salicylate	Diethyl sulfide	1.438	1.442	0.836	0.831
Methyl salicylate	1-Butanethiol	1.438	1.442	0.836	0.837
1-Chlorodecane	Mesityl oxide	1.441	1.442	0.862	0.850
Diethylene glycol	Formamide	1.445	1.446	1.128	1.129
Diethylene glycol	Ethylene glycol diglycidyl ether	1.445	1.447	1.128	1.134
Formamide	Ethylene glycol diglycidyl ether	1.446	1.447	1.129	1.134
2-Methylmorpholine	Cyclohexanone	1.446	1.448	0.951	0.943
2-Methylmorpholine	1-Amino-2-propanol	1.446	1.448	0.951	0.961
Dipropylene glycol monoethyl ether	Tetrahydrofurfuryl alcohol	1.446	1.450	1.043	1.050
1-Amino-2-methyl- 2-pentanol	2-Butylcyclohexanone	1.449	1.453	0.904	0.901
2-Propylcyclohexanone	4-Methylcyclohexanol	1.452	1.454	0.923	0.908

			ractive ndex	Density, g/mL		
Solvent 1	Solvent 2	1	2	1	2	
Carbon tetrachloride	4,5-Dichloro-1,3- dioxolan-2-one	1.459	1.461	1.584	1.591	
N-Butyldiethanolamine	Cyclohexanol	1.461	1.465	0.965	0.968	
D- α -Pinene	trans-Decahydro- naphthalene	1.464	1.468	0.855	0.867	
Propylbenzene	p-Xylene	1.490	1.493	0.858	0.857	
Propylbenzene	Toluene	1.490	1.494	0.858	0.860	
Phenyl						
1-hydroxyphenyl ether	1,3-Dimorpholy1-2- propanol	1.491	1.493	1.081	1.094	
Phenetole	Pyridine	1.505	1.507	0.961	0.978	
2-Furanmethanol	Thiophene	1.524	1.526	1.057	1.059	
m-Cresol	Benzaldehyde	1.542	1.544	1.037	1.041	

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25°C (continued)

McReynolds' Constants

The Kovats retention indices (R.I.) indicate where compounds will appear on a chromatogram with respect to unbranched alkanes injected with the sample. By definition, the R.I. for pentane is 500, for hexane is 600, for heptane is 700, and so on, regardless of the column used or the operating conditions, although the exact conditions and column must be specified, such as liquid loading, particular support used, and any pretreatment. For example, suppose that on a 20% squalane column at 100°C, the retention times for hexane. benzene, and octane are found to be 15, 16, and 25 min, respectively. On a graph of $\ln t_R^{\prime}$ (naperian logarithm of the adjusted retention time) of the alkanes versus their retention indices, a R.I. of 653 for benzene is read off the graph. The number 653 for benzene (see the last line of Table 9.8 in the column headed "1" under "Reference compounds") means that it elutes halfway between hexane and heptane on a logarithmic time scale. If the experiment is repeated with a dinonyl phthalate column, the R.I. for benzene is found to be 736 (lying between heptane and octane), which implies that dinonyl phthalate will retard benzene slightly more than squalane will; that is, dinonyl phthalate is slightly more polar than squalane by $\Delta I = 83$ units (the entry in Table 9.8 for dinonyl phthalate in the column headed "1" under "Reference compounds"). The difference gives a measure of solutesolvent interaction due to all intermolecular forces other than London dispersion forces. The latter are the principal solute–solvent effects with squalane.

Now the overall effects due to hydrogen bonding, dipole moment, acid-base properties, and molecular configuration can be expressed as

$$\sum \Delta I = ax' + by' + cz' + du' + es'$$

where $x' = \Delta I$ for benzene (the column headed "1" in Table 9.8, intermolecular forces typical of aromatics and olefins), $y' = \Delta I$ for 1-butanol (the column headed "2" in Table 9.8, electron attraction typical of alcohols, nitriles, acids, and nitro and alkyl monochlorides, dichlorides and trichlorides), $z' = \Delta I$ for 2-pentanone (the column headed "3" in Table 9.8, electron repulsion typical of ketones, ethers, aldehydes, esters, epoxides, and dimethylamino derivatives), $u' = \Delta I$ for 1-nitropropane (the column headed "4" in Table 9.8, typical of nitro and nitrile derivatives), and $s' = \Delta I$ for pyridine (or dioxane) (the column headed "5" in Table 9.8).

TABLE 9.8 McReynolds' Constants for Stationary Phases in Gas Chromatography

The McReynolds' constants listed are differences in retention index units between the reference compound run on squalane and on the other phases listed. The last entry in the table shows the absolute retention indices for the reference compounds on squalane. Reference compounds are (1) benzene, (2) 1-butanol, (3) 2-pentanone, (4) 1 nitropropane, and (5) pyridine. (Note that Rohrschneider's constants are based on these reference compounds and may differ slightly from the McReynolds' constants. The reference compounds for Rohrschneider's constants are (1) benzene, (2) ethanol, (3) 2-butanone, (4) nitromethane, and (5) pyridine.) The minimum temperature is that at which normal gas—liquid chromatography (GLC) behavior is expected. Below that temperature, the phase will be a solid or an extremely viscous gum. The maximum temperature is that above which the bleed rate will be excessive.

		Similar	Temperature, °C Reference compounds							
Liquid phase	Chemical type	liquid phases	Minimum	Maximum	1	2	3	4	5	Sum
Squalane	(2,6,10,15,19,23- Hexamethyl)tetracosane		20	150	0	0	0	0	0	0
Paraffin oil					9	5	2	6	11	33
Apolane-87	(24,24-Diethyl-19,29- dioctadecyl)hepta- tetracontane		30	280	21	10	3	12	25	71
Apiezon L			50	250	32	22	15	32	42	143
SE 30		SP-2100, SF 96	50	350	15	53	44	64	41	217
OV-101	Poly(dimethylsiloxane)	OV-1, DC 200, DC 410	50	350	17	57	45	67	43	229
OV-73	Poly(diphenyldimethylsiloxane), 5%:95%	SE 52	0	325	32	72	65	98	67	334
SE 54	Poly(diphenylvinyldimethylsiloxane), 5%:1%:94%		50	300	33	72	66	99	67	337
OV-3	Poly(diphenyldimethylsiloxane), 10%:90%		0	350	44	86	81	124	88	423
Dexsil 300	Poly(carboranemethylsiloxane)		50	500	47	80	103	148	96	474
Kel F Wax				150	55	67	114	143	116	495
Apiezon H				300	59	86	81	151	129	506

Dexsil 400	Carborane and methylphenyl-silicone		50	500	72	108	118	166	123	587
OV-7	Poly(diphenyldimethylsiloxane), 20%:80%	DC 550	20	350	69	113	111	171	128	592
Di(2-ethylhexyl) sebacate			0	125	72	168	108	180	125	653
Diisodecyl adipate				175	71	171	113	185	128	668
Decyl octyl adipate					79	179	119	193	134	704
Bis(2-ethylhexyl)- tetrachlorophthalate			0	150	112	150	123	168	181	734
Diisodecyl phthalate			0	175	84	173	137	218	155	767
Dinonyl phthalate			20	150	83	183	147	231	159	803
OV-11	Poly(diphenyldimethylsiloxane), 35%:65%	DC 710	0	350	107	149	153	228	190	827
Dioctyl phthalate			20	125	92	186	150	236	167	831
Hallcomid M-18			40	150	79	268	130	222	146	845
OV-17	Poly(diphenyldimethylsiloxane), 50%:50%		0	325	119	158	162	243	202	884
Dexsil 410	Carborane and methylcyanoethylsilicone		50	500	72	286	174	249	171	952
UCON LB-550-X			0	200	118	271	158	243	206	996
Span 80			15	150	97	266	170	216	268	1017
OV-22	Poly(diphenyldimethylsiloxane), 65%:35%		0	350	160	188	191	283	253	1075
Polypropylene glycol			0	150	128	294	173	264	226	1085
Didecyl phthalate			10	175	136	255	213	320	235	1159
OV-25	Poly(diphenyldimethylsiloxane), 75%:25%		0	350	178	204	208	305	280	1175
Polyphenyl ether OS-138 (6 rings)			0	225	182	233	228	313	293	1249
Neopentyl glycol sebacate		HI-EFF-3CP	50	225	172	327	225	344	326	1394
Squalene			0	100	152	341	328	329	344	1404
UCON 50-HB-280X			0	200	177	362	227	351	302	1419
Tricresyl phosphate			20	125	176	321	250	374	299	1420

TABLE 9.8 McReynolds' Constants for Stationary Phases in Gas Chromatography (*continued*)

		Similar liquid	Temperature, °C		Reference compounds					
Liquid phase	Chemical type	phases	Minimum	Maximum	1	2	3	4	5	Sum
Sucrose acetate isobutyrate			0	200	172	330	251	378	295	1426
QF-1			0	250	144	233	355	463	305	1500
OV-210	Poly(trifluoropropylsiloxane)	SP-2401, FS 1265	0	275	146	238	358	468	310	1520
OV-215	Poly(trifluoropropylmethyl-									
	siloxane)	XE 6O	0	275	149	240	363	478	315	1545
UCON 50-HB-2000	Emulphor ON-870		0	200	202	394	253	392	341	1582
Triton X-100	•		0	200	203	399	268	402	362	1634
UCON 50-HB-5100			0	200	214	418	278	421	375	1706
Siponate DS-10			0	200	99	569	320	344	388	1720
Tween 80			0	150	227	430	283	438	396	1747
XE-60	Poly(cyanoethylphenyl-									
	methylsiloxane)		0	250	204	381	340	493	367	1785
OV-225	Poly(cyanopropylphenyl-									
	methylsiloxane)		0	265	228	369	338	492	386	1813
Neopentyl glycol adipate		HI-EFF-3AP	50	225	232	421	311	461	424	1849
UCON 75-H-90000	Igepal CO-880		100	200	255	452	299	470	406	1882
Triton X-305			0	200	262	467	314	488	430	1961
Neopentyl glycol succinate		HI-EFF-3BP	50	230	272	469	366	539	474	2120
Igepal CO 990			100	200	298	508	345	540	475	2166
Carbowax 20M	Poly(ethylene glycol)	FFAP, SP-2300	25	275	322	536	368	572	510	2308
Epon 1001			50	225	284	489	406	539	601	2319
Carbowax 4000			60	200	325	551	375	582	520	2353
Ethylene glycol isophthalate		HI-EFF-2EP	100	225	326	508	425	607	561	2427
Ethylene glycol adipate		HI-EFF-2AP	100	225	372	576	453	655	617	2673
Butane-1,4-diol succinate		HI-EFF-4BP	50	225	369	591	457	661	629	2207
Phenyldiethanolamine		HI-EFF-10BP	0	200	386	555	472	674	654	2741
succinate										

Diethylene glycol adipate		HI-EFF-1AP, LAC- 1-R-296,	25	275	378	603	460	665	658	2764
Carbowax 1540		SP- 2330	50	175	371	639	453	666	641	2770
Hyprose SP-80			0	175	336	742	492	639	727	2936
SILAR-7CP			0	250	440	638	605	844	673	3200
ECNSS-M			30	200	421	690	581	803	732	3227
EGSS-X			90	200	484	710	585	831	778	3388
Ethylene glycol phthalate		HI-EFF-2GP	100	200	453	697	602	816	872	3410
SILAR-9CP			0	250	489	725	631	910	778	3536
SILAR-10C		SP-2340	25	275	523	757	659	942	801	3682
Diethylene glycol succinate		HI-EFF-1BP, LAC-3-R-728	20	200	499	751	593	840	860	3543
Tetrahydroxyethylenediamine		THEED	0	150	463	942	626	801	893	3725
Tetracyanoethylated		THEED	30	175	526	782	677	920	837	3742
pentaerythritol			50	173	320	762	077)20	037	3142
Ethylene glycol succinate		HI-EFF-2BP	100	200	537	787	643	903	889	3759
1,2,3,4-Tetrakis-										
(2-cyanoethoxy)butane			110	200	617	860	773	1048	941	4239
1,2,3,4,5,6-Hexakis (2			125	150	567	825	713	978	901	3984
cyanoethoxy)cyclohexane										
1,2,3-Tris-										
(2-cyanoethoxy)propane			0	175	593	857	752	1028	915	4145
N,N-Bis(2-cyanoethyl)-			0	125	690	991	853	1110	1000	4644
formamide			Ü	120	0,0		000	1110	1000	
OV-275	Dicyanoallylsilicone		25	250	781	1006	885	1177	1089	4938
0 1 2/3	Dicyanounyismeone			250	,01	1000	003	11//	1007	7730
Absolute retention index value	Absolute retention index values on squalane for reference compounds							652	699	

SECTION 10

POLYMERS, RUBBERS, FATS, OILS, AND WAXES

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10.2 SECTION 10

POLYMERS

General

Polymers are macromolecules that result from combinations of individual building blocks called monomer molecules. Most polymers are regular structures in which a single unit repeats many times. This produces a range of macromolecules that have similar structures and molecular weights. The ensemble of molecules typically exhibit average molecular weights but have characteristic properties. Polymerization of ethylene, $CH_2 = CH_2$, results in polyethylene, $CH_2 = CH_2 = CH_2$, and that "n" is a range of values. If the average chain possesses 1000 monomer units, chains having values of n such as 998, 999, 1001, 1002, etc. will be present as well. There will be more such chains near the average value and fewer or none when n is far from the average value.

In some polymers, long segments of linear polymer chains are oriented in a regular manner with respect to one another. Such polymers have many of the physical characteristics of crystals and are said to be *crystalline*. Polymers that have polar functional groups show a greater tendency to be crystalline. Orientation is aided by alignment of dipoles on different chains. Van der Waals' interactions between long hydrocarbon chains may provide sufficient total attractive energy to account for a high degree of regularity within the polymers.

Irregularities such as branch points, co-monomer units, and cross-links lead to *amorphous* polymers. These have less regular structures and typically do not have true melting points. Instead, they have glass transition temperatures at which the rigid and glass-like material becomes a viscous liquid as the temperature is raised.

Elastomers. Elastomer is a generic name for polymers that exhibit rubber-like elasticity. Elastomers are soft yet sufficiently elastic that they can usually be stretched several hundred percent under tension. When the stretching force is removed, they quickly retract and recover their original dimensions.

Polymers that soften or melt and then solidify and regain their original properties on cooling are called *thermoplastic*. A thermoplastic polymer is usually a single strand of linear polymer with few if any cross-links.

Thermosetting Polymers. Polymers that soften or melt on warming and then become infusible solids are called *thermosetting*. The term implies that thermal decomposition has not taken place. Thermosetting plastics contain a cross-linked polymer network that extends through the final material, making it stable to heat and insoluble in organic solvents. Many molded plastics are shaped while molten and are then heated further to become rigid solids of desired shapes.

Synthetic Rubbers. Synthetic rubbers are polymers with rubber-like characteristics that are prepared from dienes or olefins. Rubbers with special properties can also be prepared from other polymers, such as polyacrylates, fluorinated hydrocarbons, and polyurethanes.

Structural Differences. Polymers exhibit structural differences resulting from the type of monomer used, the polymerization method employed, and other factors. A *linear* polymer consists of long segments of single strands that are oriented in a regular manner with respect to one another. Branched polymers have substituents attached to the repeating units that extend the polymer laterally. When these units participate in chain propagation and link together chains, a cross-linked polymer is formed. A ladder polymer results when repeating units have a tetravalent structure such that a polymer consists of two backbone chains regularly cross-linked at short intervals.

Generally polymers involve bonding of the most substituted carbon of one monomeric unit to the least substituted carbon atom of the adjacent unit in a *head-to-tail* arrangement. An example is the formation of polypropylene from propylene. This is shown for three monomer units. The wavy lines indicate that more monomers would lead to extended chains.

$$H_3C$$
 + H_3C + H_3C + H_3C - H_3C

Substituents appear on alternate carbon atoms. *Tacticity* refers to the configuration of substituents relative to the backbone axis. In an *isotactic* arrangement, substituents are on the same plane of the backbone axis; that is, the configuration at each chiral center is identical.

In a *syndiotactic* arrangement, the substituents are in an ordered alternating sequence, appearing alternately on one side and then on the other side of the chain, as shown for a segment of a vinyl chloride polymer. If the sidechains are not in any particular order with respect to each other (random), the polymer is said to be *atactic*.

Copolymerization. Copolymerization occurs when a mixture of two or more monomer types polymerizes so that each kind of monomer enters the polymer chain. The fundamental structure resulting from copolymerization depends on the nature of the monomers and the relative rates of monomer reactions with the growing polymer chain. A tendency toward alternation of monomer units is common. Random copolymerization is known but it is rather unusual.

$$A = A = A = A = A = A = A = B$$

In *graft copolymers* the chain backbone is composed of one kind of monomer and the branches are made up of another kind of monomer. The structure of a *block copolymer* consists of a homopolymer attached to chains of another homopolymer. In either case, cis or trans (Z or E) double bond configurations around any double bond not involved in the polymerization will normally be unaltered.

Schematic of a graft copolymer

Schematic of a block copolymer

10.4 SECTION 10

Dendrimers

A relatively recent development in polymer chemistry is the family of compounds known as dendrimers. The term derives from the Greek *dendra* meaning tree. Tree-like structures of this general type have also been referred to as arborols. Dendrimers differ from typical polymers in that they radiate from a central unit or core rather than being either linear or planar. Dendrimers are built up using a "generational" structure in discrete synthetic steps. As a result, the product is nearer to being a single compound than is a typical polymer. A typical dendrimer consists of a multifunctional core unit. Each functional group of the core unit is elaborated by a further molecular unit, often referred to as a "dendritic wedge." The core unit is usually designated "generation 0" and additional units radiating from it or prior units are designated as higher generations, that is, generation 1, generation 2, etc. When the synthesis begins at the core and radiates outward, it is called a divergent synthesis. Alternately, synthesis may begin at the outside and terminate with a core unit.

The more common divergent method is illustrated in the following scheme. 1,3,5-Tricarboxybenzene (trimesic acid) serves as the core or generation 0. It could be functionalized by converting it into the tris(acid chloride). Reaction with the secondary amine of diethanolamine would give the tris(amide) hexahydroxy compound shown here. This structure represents generations 0 and 1. Treatment with an appropriately substituted benzyl chloride could lead to the hexaether that comprises generations 0, 1, and 2. There are now a dozen "Y" groups that could be further functionalized in going to generation 3. A difficulty is that the functional or protecting groups present at each stage must be compatible with the chemistry used to make the connections.

A second issue is that when subsequent generations involve sterically demanding structural units, incomplete substitution may occur. Thus, in the final structure shown, five

benzyl ethers might form, rather than six, owing to steric crowding. This would introduce a defect in the dendrimer structure. Indeed, some molecules might possess all six benzyl ethers whereas others might lack one or even two. It must be possible to manipulate the substituents designated "Y" in the presence of ether and amide groups to further extend the dendrimer.

Novel dendrimers have novel and unique properties that make them promising candidates for use in the development of nanoscale devices and in drug delivery systems.

Additives to Polymers

Antioxidants. Antioxidants markedly retard the rate of autoxidation throughout the useful life of the polymer. Chain-terminating antioxidants have a reactive —NH or —OH functional group and include compounds such as secondary aryl amines or hindered phenols. They function by transfer of hydrogen to free radicals, principally to peroxy radicals. Butylated hydroxytoluene is a widely used example.

Peroxide-decomposing antioxidants destroy hydroperoxides, the sources of free radicals in polymers. Phosphites and thioesters such as tris(nonylphenyl) phosphite, distearyl pentaerythritol diphosphite, and dialkyl thiodipropionates are examples of peroxide-decomposing antioxidants.

Antistatic Agents. External antistatic agents are usually quaternary ammonium salts of fatty acids and ethoxylated glycerol esters of fatty acids that are applied to the plastic surface. Internal antistatic agents are compounded into plastics during processing. Carbon blacks provide a conductive path through the bulk of the plastic. Other types of internal agents must bloom to the surface after compounding in order to be active. These latter materials are ethoxylated fatty amines and ethoxylated glycerol esters of fatty acids, which often must be individually selected to match chemically each plastic type.

Antistatic agents require ambient moisture to function. Consequently their effectiveness is dependent on the relative humidity. They provide a broad range of protection at 50% relative humidity. Much below 20% relative humidity, only materials that provide a conductive path through the bulk of the plastic to ground (such as carbon black) will reduce electrostatic charging.

Chain-Transfer Agents. Chain-transfer agents are used to regulate the molecular weight of polymers. These agents react with the developing polymer and interrupt the growth of a particular chain. The products, however, are free radicals that are capable of adding to monomers and initiating the formation of new chains. The overall effect is to reduce the average molecular weight of the polymer without reducing the rate of polymerization. Branching may occur as a result of chain transfer between a growing but rather short chain with another and longer polymer chain. Branching may also occur if the radical end of a growing chain abstracts a hydrogen atom from a carbon atom four or five carbons removed from the end. Thiols are commonly used as chain-transfer agents.

Coupling Agents. Coupling agents are molecular bridges between the interface of an inorganic surface (or filler) and an organic polymer matrix. Titanium-derived coupling agents interact with the free protons at the inorganic interface to form organic monomolecular layers on the inorganic surface. The titanate-coupling-agent molecule has six functions:

$$(RO)_m$$
 — Ti — $(O - Y - R^1 - Z)_m$

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where

Туре	m	n
Monoalkoxy	1	3
Coordinate	4	2
Chelate	1	2

Function 1 is the attachment of the hydrolyzable portion of the molecule to the surface of the inorganic (or proton-bearing) species.

Function 2 is the ability of the titanate molecule to transesterify.

Function 3 affects performance as determined by the chemistry of alkylate, carboxyl, sulfonyl, phenolic, phosphate, pyrophosphate, and phosphite groups.

Function 4 provides van der Waals' entanglement via long carbon chains.

Function 5 provides thermoset reactivity via functional groups such as methacrylates and amines.

Function 6 permits the presence of two or three pendent organic groups. This allows all functionality to be controlled to the first-, second-, or third-degree levels.

Silane coupling agents are represented by the formula

$$Z-R-SiY_3$$

where Y represents a hydrolyzable group (typically alkoxy); Z is a functional organic group, such as amino, methacryloxy, epoxy; and R typically is a short aliphatic linkage that serves to attach the functional organic group to silicon in a stable fashion. Bonding to surface hydroxy groups of inorganic compounds is accomplished by the —SiY₃ portion, either by direct bonding of this group or more commonly via its hydrolysis product —Si(OH)₃. Subsequent reaction of the functional organic group with the organic matrix completes the coupling reaction and establishes a covalent chemical bond from the organic phase through the silane coupling agent to the inorganic phase.

Flame Retardants. Flame retardants are thought to function via several mechanisms, dependent upon the class of flame retardant used. Halogenated flame retardants are thought to function principally in the vapor phase either as a diluent and heat sink or as a free-radical trap that stops or slows flame propagation. Phosphorus compounds are thought to function in the solid phase by forming a glaze or coating over the substrate that prevents the heat and mass transfer necessary for sustained combustion. With some additives, as the temperature is increased, the flame retardant acts as a solvent for the polymer, causing it to melt at lower temperatures and flow away from the ignition source.

Mineral hydrates, such as alumina trihydrate and magnesium sulfate heptahydrate, are used in highly filled thermosetting resins.

Foaming Agents (Chemical Blowing Agents). Foaming agents are added to polymers during processing to form minute gas cells throughout the product. Physical foaming agents include liquids and gases. Compressed nitrogen is often used in injection molding. Common liquid foaming agents are short-chain aliphatic hydrocarbons in the C_5 to C_7 range and their chlorinated or fluorinated analogs.

The chemical foaming agent used varies with the temperature employed during processing. At relatively low temperatures $(15-200\,^{\circ}\text{C})$, the foaming agent is often 4,4'-oxybis(benzenesulfonylhydrazide) or *p*-toluenesulfonylhydrazide. In the midrange $(160-232\,^{\circ}\text{C})$, either sodium hydrogen carbonate or 1,1'azobisformamide is used. For the

high range (200–285°C), there are p-toluenesulfonylsemicarbazide, 5-phenyltetrazole and analogs, and trihydrazinotriazine.

Inhibitors. Inhibitors slow or stop polymerization by reacting with the initiator or the growing polymer chain. The free radical formed from an inhibitor must be sufficiently unreactive that it does not function as a chain-transfer agent and begin another growing chain. Benzoquinone is a typical free-radical chain inhibitor. The resonance-stabilized free radical usually dimerizes or disproportionates to produce inert products and end the chain process.

Lubricants. Materials such as fatty acids are added to reduce the surface tension and improve the handling qualities of plastic films.

Plasticizers are relatively nonvolatile liquids which are blended with polymers Plasticizers. to alter their properties by intrusion between polymer chains. Diisooctyl phthalate is a common plasticizer. A plasticizer must be compatible with the polymer to avoid bleeding out over long periods of time. Products containing plasticizers tend to be more flexible and workable.

Ultraviolet Stabilizers. 2-Hydroxybenzophenones represent the largest and most versatile class of ultraviolet stabilizers that are used to protect materials from the degradative effects of ultraviolet radiation. They function by absorbing ultraviolet radiation and by quenching electronically excited states.

Hindered amines, such as 4-(2,2,6,6-tetramethylpiperidinyl) decanedioate, serve as radical scavengers and will protect thin films under conditions in which ultraviolet absorbers are ineffective. Metal salts of nickel, such as dibutyldithiocarbamate, are used in polyolefins to quench singlet oxygen or electronically excited states of other species in the polymer. Zinc salts function as peroxide decomposers.

Vulcanization and Curing. Originally, vulcanization implied heating natural rubber with sulfur, but the term is now also employed for curing polymers. When sulfur is employed, sulfide and disulfide cross-links form between polymer chains. This provides sufficient rigidity to prevent plastic flow. Plastic flow is a process in which coiled polymers slip past each other under an external deforming force; when the force is released, the polymer chains do not completely return to their original positions.

Organic peroxides are used extensively for the curing of unsaturated polyester resins and the polymerization of monomers having vinyl unsaturation. The -O-O bond is split into free radicals which can initiate polymerization or cross-linking of various monomers or polymers.

TABLE 10.1 Plastic Families

Acetals

Acrylics

Poly(methyl methacrylate) (PMMA) Poly(acrylonitrile)

Alkyds

Alloys

Acrylic-poly(vinyl chloride) alloy Acrylonitrile-butadiene-styrenepoly(vinyl chloride) alloy (ABS-PVC) Acrylonitrile-butadiene-styrenepolycarbonate alloy (ABS-PC)

Allyls

Allyl-diglycol-carbonate polymer Diallyl phthalate (DAP) polymer

Cellulosics

Cellulose acetate resin

Cellulose-acetate-propionate resin

Cellulose-acetate-butyrate resin

Cellulose nitrate resin

Ethyl cellulose resin

Rayon

Chlorinated polyether

Epoxy

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TABLE 10.1 Plastic Families (*continued*)

Fluorocarbons

Poly (tetrafluoroethylene) (PTFE)

Poly (chlorotrifluoroethylene) (PCTFE)

Perfluoroalkoxy (PFA) resin

Fluorinated ethylene-propylene (FEP)

resin

Poly(vinylidene fluoride) (PVDF)

Ethylene-chlorotrifluoroethylene

copolymer

Ethylene–tetrafluoroethylene copolymer Poly(vinyl fluoride) (PVF)

Melamine formaldehyde

Melamine phenolic

Nitrile resins

Phenolics

Polyamides

Nylon 6

Nvlon 6/6

Nylon 6/9

Nylon 6/12

Nylon 11

Nylon 12

Aromatic nylons

Poly(amide-imide)

Poly(aryl ether)

Polycarbonate (PC)

Polyesters

Poly(butylene terephthalate) (PBT)

[also called polytetramethylene

terephthalate (PTMT)]

Poly(ethylene terephthalate) (PET)

Unsaturated polyesters (SMC, BMC)

Butadiene–maleic acid copolymer (BMC) Styrene–maleic acid copolymer (SMC)

Polvimide

Poly(methylpentene)

Polyolefins (PO)

Low-density polyethylene (LDPE)

High-density polyethylene (HDPE)

Ultrahigh-molecular-weight polyethylene

(UHMWPE)

Polypropylene (PP)

Polybutylene (PB)

Polyallomers

Poly(phenylene oxide)

Poly(phenylene sulfide) (PPS)

Polyurethanes

Silicones

Styrenics

Polystyrene (PS)

Acrylonitrile-butadiene-styrene (ABS)

copolymer

Sytrene-acrylonitrile (SAN) copolymer

Styrene-butadiene copolymer

Sulfones

Polysulfone (PSF)

Poly(ether sulfone)

Poly(phenyl sulfone)

Thermoplastic elastomers

Polvolefin

Polyester

Block copolymers

Styrene-butadiene block copolymer

Styrene-isoprene block copolymer

Styrene-ethylene block copolymer

Styrene–butylene block copolymer

Urea formaldehyde

Vinyls

Poly(vinyl chloride) (PVC)

Poly(vinyl acetate) (PVAC)

Poly(vinylidene chloride)

Poly(vinyl butyrate) (PVB)

Tory (viny) butyrate) (1 v

Poly(vinyl formal)

Poly(vinyl alcohol) (PVAL)

FORMULAS AND KEY PROPERTIES OF PLASTIC MATERIALS

Acetals

Homopolymer. Acetal homopolymers are prepared from formaldehyde and consist of high-molecular-weight linear polymers of formaldehyde. The trimer of formaldehyde is shown to the left and the structure of the polymer is shown at the right, below.

$$\begin{array}{ccc}
 & & & H \\
 & & \downarrow \\
 &$$

The good mechanical properties of this homopolymer result from the ability of the oxymethylene chains to pack together into a highly ordered crystalline configuration as the polymers change from the molten to the solid state.

Key properties include high melt point, strength and rigidity, good frictional properties, and resistance to fatigue. Higher molecular weight increases toughness but reduces melt flow.

Copolymer. Acetal copolymers are prepared by copolymerization of 1,3,5-trioxane with small amounts of a co-monomer. Carbon–carbon bonds are distributed randomly in the polymer chain. These carbon–carbon bonds help to stabilize the polymer against thermal, oxidative, and acidic attack.

Acrylics

Poly(methyl methacrylate). Acrylic acid is H_2C =CH—COOH and methacrylic acid is H_2C =C(CH₃)COOH. These compounds and their methyl esters are both quite reactive and difficult to store and handle. The monomer used to form poly(methyl methacrylate), 2-hydroxy-2-methylpropanenitrile, is prepared by the following reaction:

$$\begin{array}{c} OH \\ CH_3-C-CH_3+HCN \rightarrow CH_3-C-CH_3 \\ O \\ O \\ CN \end{array}$$

2-Hydroxy-2-methylpropanenitrile is then reacted with methanol (or other alcohol) to yield methacrylate ester. Free-radical polymerization is initiated by peroxide or azo catalysts and produce poly(methyl methacrylate) resins having the following formula:

$$\begin{bmatrix} CH_3 \\ -CH_2 - C - \\ COOCH_3 \end{bmatrix}_n$$

Key properties are good resistance to heat, light, and weathering. This polymer is unaffected by most detergents, cleaning agents, and solutions of inorganic acids, alkalies, and aliphatic hydrocarbons. Poly(methyl methacrylate) has light transmittance of 92% with a haze of 1–3% and its clarity is equal to glass.

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Poly(methyl acrylate). The structure of methyl acrylate is $H_2C = CH - COOCH_3$. The monomer used to prepare poly(methyl acrylate) is produced by the oxidation of propylene. The resin is made by free-radical polymerization initiated by peroxide catalysts and has the following formula:

$$\begin{bmatrix} -CH_2 - CH - \\ COOCH_3 \end{bmatrix}_n$$

Poly(methyl acrylate) resins vary from soft, elastic, film-forming materials to hard plastics.

Poly(acrylic acid) and Poly(methacrylic acid). Glacial acrylic acid and glacial methacrylic acid can be polymerized to produce water-soluble polymers having the following structures:

$$\begin{bmatrix} -CH_2 - CH - \\ COOH \end{bmatrix}_n \begin{bmatrix} CH_3 \\ -CH_2 - C - \\ COOH \end{bmatrix}_n$$

These monomers provide a means for introducing carboxyl groups into copolymers. In copolymers these acids can improve adhesion properties, improve freeze—thaw and mechanical stability of polymer dispersions, provide stability in alkalies (including ammonia), increase resistance to attack by oils, and provide reactive centers for cross-linking by divalent metal ions, diamines, or epoxides.

Functional Group Methacrylate Monomers. Hydroxyethyl methacrylate and dimethylaminoethyl methacrylate produce polymers having the following formulas:

$$\begin{bmatrix} \operatorname{CH_3} & \operatorname{CH_3} \\ -\operatorname{CH_2-C-} & \\ \operatorname{COOCH_2CH_2OH} \end{bmatrix}_n \quad \begin{bmatrix} \operatorname{CH_3} \\ -\operatorname{CH_2-C-} \\ \operatorname{COOCH_2CH_2N(CH_3)_2} \end{bmatrix}_n$$

The use of hydroxyethyl (also hydroxypropyl) methacrylate as a monomer permits the introduction of reactive hydroxyl groups into the copolymers. This offers the possibility for subsequent cross-linking with an HO-reactive diffunctional agent (diisocyanate, diepoxide, or melamineformaldehyde resin). Hydroxyl groups promote adhesion to polar substrates.

Use of dimethylaminoethyl (also *tert*-butylaminoethyl) methacrylate as a monomer permits the introduction of pendent amino groups which can serve as sites for secondary crosslinking, provide a way to make the copolymer acid-soluble, and provide anchoring sites for dyes and pigments.

Poly(acrylonitrile). Acrylonitrile has the formula $H_2C = CH - C \equiv N$. Poly(acrylonitrile) polymers have the following formula:

$$\begin{bmatrix} -CH_2 - CH - \\ | \\ | \\ CN \end{bmatrix}_n$$

Alkyds

Alkyds are formulated from polyester resins, cross-linking monomers, and fillers of mineral or glass. The unsaturated polyester resins used for thermosetting alkyds are the reaction products of polyfunctional organic alcohols (glycols) and dibasic organic acids. Key properties of alkyds are dimensional stability, colorability, and arc track resistance. Chemical resistance, however, is generally poor.

Alloys

Polymer alloys are physical mixtures of structurally different homopolymers or copolymers. The mixture is held together by secondary intermolecular forces such as dipole interaction, hydrogen bonding, or van der Waals' forces.

Homogeneous alloys have a single glass transition temperature which is determined by the ratio of the components. The physical properties of these alloys are averages based on the composition of the alloy. Heterogeneous alloys can be formed when graft or block copolymers are combined with a compatible polymer. Alloys of incompatible polymers can be formed if an interfacial agent can be found.

Allyls

Diallyl Phthalate (and Diallyl 1,3-Phthalate). Phthalic acid is 1,2-dicarboxybenzene. The 1,3-isomer is generally referred to as isophthalic acid. These allyl polymers are prepared from

These resulting polymers are solid, linear, internally cyclized, thermoplastic structures containing unreacted allylic groups spaced at regular intervals along the polymer chain. Compounds derived from these polymers that are molded with mineral, glass, or synthetic fiber filling exhibit good electrical properties under high humidity and high temperature conditions. They also show stable low-loss factors, high surface and volume resistivity, and high arc and track resistance.

Cellulosics

Cellulose Triacetate. Cellulose triacetate is prepared according to the following reaction:

$$CH_3-C$$
 CH_3-C
 CH_3-C
 CH_3-C
 CH_3-C
 CH_3-C
 CH_3-C
 CH_3-C

Because cellulose triacetate has a high softening temperature, it must be processed in solution. A mixture of dichloromethane and methanol is a common solvent.

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Cellulose triacetate sheeting and film have good gauge uniformity and good optical clarity. Cellulose triacetate products have good dimensional stability and resistance to water and have good folding endurance and burst strength. It is highly resistant to solvents such as acetone. Cellulose triacetate products have good heat resistance and a high dielectric constant.

Cellulose Acetate, Propionate, and Butyrate. Cellulose acetate is prepared by hydrolyzing the triester to remove some of the acetyl groups; the plastic-grade resin contains 38–40% acetyl. The propionate and butyrate esters are made by substituting propionic acid and its anhydride (or butyric acid and its anhydride) for some of the acetic acid and acetic anhydride. Plastic grades of cellulose-acetate–propionate resin contain 39–47% propionyl and 2–9% acetyl; cellulose-acetate–butyrate resins contain 26–39% butyryl and 12–15% acetyl.

These cellulose esters form tough, strong, stiff, hard plastics with almost unlimited color possibilities. Articles made from these plastics have a high gloss and are suitable for use in contact with food.

Cellulose Nitrate. Cellulose nitrate is prepared according to the following reaction:

$$C_6H_{10}O_5 + HNO_3 \rightarrow [-C_6H_7O_2(OH)(ONO_2)_2 -]_n$$

The nitrogen content for plastics is usually about 11%, for lacquers and cement base it is 12%, and for explosives it is 13%. The standard plasticizer added is camphor.

Key properties of cellulose nitrate are good dimensional stability, low water absorption, and toughness. Its disadvantages are its flammability and lack of stability to heat and sunlight.

Ethyl Cellulose. Ethyl cellulose is prepared by reacting cellulose with caustic to form caustic cellulose, which is then reacted with chloroethane to form ethyl cellulose. Plastic-grade material contains 44–48% ethoxyl.

Although not as resistant as cellulose esters to acids, it is much more resistant to bases. An outstanding feature is its toughness at low temperatures.

Rayon. Viscose rayon is obtained by reacting the hydroxy groups of cellulose with carbon disulfide in the presence of alkali to give xanthates. When this solution is poured (spun) into an acid medium, the reaction is reversed and the cellulose is regenerated (coagulated).

Ероху

Epoxy resin is prepared by the following condensation reaction:

$$CH_2-CH-CH_2 \xrightarrow{CH_3} OH \\ -C \xrightarrow{CH_2-CH-CH_2} O-CH_2-CH-CH_2 \xrightarrow{R}$$

The condensation leaves epoxy end groups that are then reacted in a separate step with nucleophilic compounds (alcohols, acids, or amines). For use as an adhesive, the epoxy

resin and the curing resin (usually an aliphatic polyamine) are packaged separately and mixed together immediately before use.

Epoxy novolac resins are produced by glycidation of the low-molecular-weight reaction products of phenol (or cresol) with formaldehyde. Highly cross-linked systems are formed that have superior performance at elevated temperatures.

Fluorocarbon

Poly(tetrafluoroethylene). Poly(tetrafluoroethylene) is prepared from tetrafluoroethylene and consists of repeating units in a predominantly linear chain:

$$F_2C = CF_2 \rightarrow [-CF_2 - CF_2 -]_n$$

Tetrafluoroethylene polymer has the lowest coefficient of friction of any solid. It has remarkable chemical resistance and a very low brittleness temperature $(-100\,^{\circ}\text{C})$. Its dielectric constant and loss factor are low and stable across a broad temperature and frequency range. Its impact strength is high.

Fluorinated Ethylene–Propylene Resin. Polymer molecules of fluorinated ethylene-propylene consist of predominantly linear chains with this structure:

$$\begin{bmatrix} -\operatorname{CF}_2 - \operatorname{CF}_2 - \operatorname{CF}_2 - \operatorname{CF} - \\ | & | \\ \operatorname{CF}_3 \end{bmatrix}_n$$

Key properties are its flexibility, translucency, and resistance to all known chemicals except molten alkali metals, elemental fluorine and fluorine precursors at elevated temperatures, and concentrated perchloric acid. It withstands temperatures from -270° to 250° C and may be sterilized repeatedly by all known chemical and thermal methods.

Perfluoroalkoxy Resin. Perfluoroalkoxy resin has the following formula:

$$\begin{bmatrix} -\operatorname{CF}_2 - \operatorname{CF}_2 - \operatorname{CF}_2 - \operatorname{CF}_2 - \operatorname{CF}_2 - \\ 0 \\ 0 \\ R \end{bmatrix}_n$$
 where R is $-\operatorname{C}_n\operatorname{F}_{2n+1}$

It resembles polytetrafluoroethylene and fluorinated ethylene propylene in its chemical resistance, electrical properties, and coefficient of friction. Its strength, hardness, and wear resistance are about equal to the former plastic and superior to that of the latter at temperatures above 150 °C.

Poly(vinylidene fluoride). Poly(vinylidene fluoride) consists of linear chains in which the predominant repeating unit is

$$[-CH_2-CF_2-]_n$$

It has good weathering resistance and does not support combustion. It is resistant to most chemicals and solvents and has greater strength, wear resistance, and creep resistance than the preceding three fluorocarbon resins.

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Poly(1-chloro-1,2,2-trifluoroethylene). Poly(1-chloro-1,2,2-trifluoroethylene consists of linear chains in which the predominant repeating unit is

$$\begin{bmatrix} -CF_2 - CF - \\ | \\ | \\ | \end{bmatrix}$$

It possesses outstanding barrier properties to gases, especially water vapor. It is surpassed only by the fully fluorinated polymers in chemical resistance. A few solvents dissolve it at temperatures above 100°C, and it is swollen by a number of solvents, especially chlorinated solvents. It is harder and stronger than perfluorinated polymers, and its impact strength is lower.

Ethylene–Chlorotrifluoroethylene Copolymer. Ethylene–chlorotrifluoroethylene copolymer consists of linear chains in which the predominant 1:1 alternating copolymer is

$$\begin{bmatrix} -CH_2 - CH_2 - CF_2 - CF_- \\ Cl \end{bmatrix}_n$$

This copolymer has useful properties from cryogenic temperatures to 180°C. Its dielectric constant is low and stable over a broad temperature and frequency range.

Ethylene-Tetrafluoroethylene Copolymer. Ethylene-tetrafluoroethylene copolymer consists of linear chains in which the repeating unit is

$$[-CH_2-CH_2-CF_2-CF_2-]_n$$

Its properties resemble those of ethylene-chlorotrifluoroethylene copolymer.

Poly(vinyl fluoride). Poly(vinyl fluoride) consists of linear chains in which the repeating unit is

$$[-CH2-CHF-]_n$$

It is used only as a film, and it has good resistance to abrasion and resists staining. It also has outstanding weathering resistance and maintains useful properties from -100 to 150 °C.

Nitrile Resins

The principal monomer of nitrile resins is acrylonitrile (see "Polyacrylonitrile"), which constitutes about 70% by weight of the polymer and provides the polymer with good gas barrier and chemical resistance properties. The remainder of the polymer is 20–30% methyl acrylate (or styrene), with 0–10% butadiene to serve as an impact-modifying termonomer.

Melamine Formaldehyde

The monomer used for preparing melamine formaldehyde is formed as follows:

Hexamethylolmelamine

Hexamethylolmelamine can further condense in the presence of an acid catalyst; ether linkages can also form (see "Urea Formaldehyde"). A wide variety of resins can be obtained by careful selection of pH, reaction temperature, reactant ratio, amino monomer, and extent of condensation. Liquid coating resins are prepared by reacting methanol or butanol with the initial methylolated products. These can be used to produce hard, solvent-resistant coatings by heating with a variety of hydroxy, carboxyl, and amide functional polymers to produce a cross-linked film.

Phenolics

Phenol-formaldehyde resin. Phenol-formaldehyde resin is prepared from phenol by reaction with formaldehyde. Phenol is an enol, the 2-, 4-, and 6-positions of which are activated for reaction with an electrophile. Phenol is sequentially hydroxymethylated approximately as illustrated below. Dehydration of the phenolic hydroxymethyl groups affords a benzyl cation, a new electrophile that can react with another substituted or unsubstituted molecule of phenol. Both linear polymerization and cross-linking are possible, depending on the ratio of the reactants and the polymerization conditions.

$$\overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\overset{\mathsf{OH}}} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\longleftarrow} \overset{\mathsf{OH}}{\overset{$$

One-Stage Resins. The ratio of formaldehyde to phenol is high enough to allow the thermosetting process to take place without the addition of other sources of cross-links.

Two-Stage Resins The ratio of formaldehyde to phenol is low enough to prevent the thermosetting reaction from occurring during manufacture of the resin. At this point the resin is termed *novolac* resin. Subsequently, hexamethylenetetramine is incorporated into the material to act as a source of chemical cross-links during the molding operation (and conversion to the thermoset or cured state).

Polyamides

Nylon 6, 11, and 12. This class of polymers is polymerized by addition reactions of ring compounds that contain both acid and amine groups on the monomer.

Nylon 6 is polymerized from 2-oxohexamethyleneimine (6 carbons); nylon 11 and 12 are made this way from 11- and 12-carbon rings, respectively.

Nylon 6/6, 6/9, and 6/12. As illustrated below, nylon 6/6 is polymerized from 1,6-hexanedioic acid (six carbons) and 1,6-hexanediamine (six carbons).

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$$HOOC$$
— $(CH_2)_4$ — $COOH + H_2N$ — CH_2 — $(CH_2)_4$ — CH_2 — NH_2

1.6-Hexanedioic acid

1.6-Hexanediamine

$$\begin{bmatrix} -NH - (CH_2)_6 - NH - C - (CH_2)_4 - C - \\ \parallel & \parallel \\ O & O \end{bmatrix}$$

Poly(hexamethylene 1,6- hexanediamide)

Other nylons are made this way from different combinations of monomers to produce types 6/9, 6/10, and 6/12.

Nylon 6 and 6/6 possess the maximum stiffness, strength, and heat resistance of all the types of nylon. Type 6/6 has a higher melt temperature, whereas type 6 has a higher impact resistance and better processibility. At a sacrifice in stiffness and heat resistance, the higher analogs of nylon are useful primarily for improved chemical resistance in certain environments (acids, bases, and zinc chloride solutions) and for lower moisture absorption.

Aromatic nylons, $[-NH-C_6H_4-CO-]_n$, (also called aramids) have specialty uses because of their improved clarity.

Poly (amide-imide)

Poly(amide-imide) is the condensation polymer of 1,2,4-benzenetricarboxylic anhydride and various aromatic diamines and has the general structure:

$$\begin{bmatrix} H & & & & \\ & & & & \\ -R-N-C & & & & \\ & & & & \\ 0 & & & & \\ \end{bmatrix}$$

It is characterized by high strength and good impact resistance, and retains its physical properties at temperatures up to to 260 °C. Its radiation (gamma) resistance is good.

Polycarbonate

Polycarbonate is a polyester in which dihydric (or polyhydric) phenols are joined through carbonate linkages. The general-purpose type of polycarbonate is based on 2,2-bis(4'-hydroxybenzene) propane (bisphenol A) and has the general structure:

Polycarbonates are the toughest of all thermoplastics. They are window-clear, amazingly strong and rigid, autoclavable, and nontoxic. They have a brittleness temperature of $-135\,^{\circ}\mathrm{C}$.

Polyester

Poly(butylene terephthalate). Poly(butylene terephthalate) is prepared in a condensation reaction between dimethyl terephthalate and 1,4-butanediol and its repeating unit has the general structure

This thermoplastic shows good tensile strength, toughness, low water absorption, and good frictional properties, plus good chemical resistance and electrical properties.

Poly(ethylene terephthalate). Poly(ethylene terephthalate) is prepared by the reaction of either terephthalic acid or dimethyl terephthalate with ethylene glycol, and its repeating unit has the general structure

The resin has the ability to be oriented by a drawing process and crystallized to yield a high-strength product.

Unsaturated Polyesters. Unsaturated polyesters are produced by reaction between two types of dibasic acids, one of which is unsaturated, and an alcohol to produce an ester. Double bonds in the body of the unsaturated dibasic acid are obtained by using maleic anhydride or fumaric acid.

PCTA Copolyester. Poly(1,4-cyclohexanedimethylene terephthalic acid) (PCTA) copolyester is a polymer of cyclohexanedimethanol and terephthalic acid, with another acid substituted for a portion of the terephthalic acid otherwise required. It has the following formula:

$$\begin{bmatrix} -O-CH_2 & O & O \\ -CH_2-O-C & -C- \end{bmatrix}$$

Polyimides. Polyimides have the following formula:

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They are used as high-temperature structural adhesives since they become rubbery rather than melt at about 300°C.

Poly(methylpentene)

Poly(methylpentene) is obtained by a Ziegler-type catalytic polymerization of 4-methyl-1-pentene.

Its key properties are its excellent transparency, rigidity, and chemical resistance, plus its resistance to impact and to high temperatures. It withstands repeated autoclaving, even at 150°C.

Polyolefins

Polyethylene. Polymerization of ethylene results in an essentially straight-chain high-molecular-weight hydrocarbon.

$$CH_2 = CH_2 \rightarrow [-CH_2 - CH_2 -]_n$$

Branching occurs to some extent and can be controlled. Minimum branching results in a "high-density" polyethylene because of its closely packed molecular chains. More branching gives a less compact solid known as "low-density" polyethylene.

A key property is its chemical inertness. Strong oxidizing agents eventually cause some oxidation, and some solvents cause softening or swelling, but there is no known solvent for polyethylene at room temperature. The brittleness temperature is -100° C for both types. Polyethylene has good low-temperature toughness, low water absorption, and good flexibility at subzero temperatures.

Polypropylene. The polymerization of propylene results in a polymer with the following structure:

$$CH_2=CH-CH_3 \rightarrow \begin{bmatrix} -CH_2-CH-\\ CH_3 \end{bmatrix}_{II}$$

The desired form in homopolymers is the isotactic arrangement (at least 93% is required to give the desired properties). Copolymers have a random arrangement. In block copolymers a secondary reactor is used where active polymer chains can further polymerize to produce segments that use ethylene monomer.

Polypropylene is translucent and autoclavable and has no known solvent at room temperature. It is slightly more susceptible to strong oxidizing agents than polyethylene.

Polybutylene. Polybutylene is composed of linear chains having an isotactic arrangement of ethyl side groups along the chain backbone.

$$CH_2 = CH - CH_2 - CH_3 \rightarrow \begin{bmatrix} -CH_2 - CH - \\ CH_2 \\ CH_2 \\ CH_3 \end{bmatrix}_n$$

It has a helical conformation in the stable crystalline form.

Polybutylene exhibits high tear, impact, and puncture resistance. It also has low creep, excellent chemical resistance, and abrasion resistance with coilability.

Ionomer. Ionomer is the generic name for polymers based on sodium or zinc salts of ethylene–methacrylic acid copolymers in which interchain ionic bonding, occurring randomly between the long-chain polymer molecules, produces solid-state properties.

The abrasion resistance of ionomers is outstanding, and ionomer films exhibit optical clarity. In composite structures ionomers serve as a heat-seal layer.

Poly(phenylene sulfide)

Poly(phenylene sulfide) has the following formula:

$$\begin{bmatrix} - \\ - \end{bmatrix}_n$$

The recurring *para*-substituted benzene rings and sulfur atoms form a symmetrical rigid backbone.

The high degree of crystallization and the thermal stability of the bond between the benzene ring and sulfur are the two properties responsible for the polymer's high melting point, thermal stability, inherent flame retardance, and good chemical resistance. There are no known solvents of poly(phenylene sulfide) that can function below 205 °C.

Polyurethane

Foams. Polyurethane foams are prepared by the polymerization of polyols with isocyanates. One of the most commonly used reactive isocyanates toluenediisocyanate, TDI. It is made from toluene by nitration and then reduction followed by treatment with phosgene. The isocyanate residue reacts readily with alcohols to give carbamates (urethanes) or amines to give ureas.

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Commonly used isocyanates are toluenediisocyanate, methylenediphenylisocyanate, and polymeric isocyanates. Polyols used are macroglycols based on either polyester or polyether. The former [poly(ethylene phthalate) or poly(ethylene 1,6-hexanedioate)] have hydroxyl groups that are free to react with the isocyanate. Most flexible foam is made from 80/20 toluene diisocyanate (which refers to the ratio of 2,4-toluenediisocyanate to 2,6-toluene diisocyanate). High-resilience foam contains about 80% 80/20 toluenediisocyanate and 20% poly(methylene diphenyl isocyanate), while semiflexible foam is almost always 100% poly(methylene diphenyl isocyanate). Much of the latter reacts by trimerization to form isocyanurate rings.

Flexible foams are used in mattresses, cushions, and safety applications. Rigid and semiflexible foams are used in structural applications and to encapsulate sensitive components to protect them against shock, vibration, and moisture. Foam coatings are tough, hard, flexible, and chemically resistant.

Elastomeric Fiber. Elastomeric fibers are prepared by the polymerization of polymeric polyols with disocyanates.

toluenediisocyanate

The structure of elastomeric fibers is similar to that illustrated for polyurethane foams.

SILICONES

Silicones are formed in the following multistage reaction:

$$\begin{array}{c} R_2SiCl_2 + 2H_2O \rightarrow R_2Si(OH)_2 + 2HCl \\ \downarrow \\ [-Si(R)_2 - O -]_n \end{array}$$

The silanols formed above are unstable and undergo dehydration. On polycondensation, they give polysiloxanes (or silicones) which are characterized by their three-dimensional branched-chain structure. Various organic groups introduced within the polysiloxane chain impart certain characteristics and properties to these resins.

Methyl groups impart water repellency, surface hardness, and noncombustibility.

Phenyl groups impart resistance to temperature variations, flexibility under heat, resistance to abrasion, and compatibility with organic products.

Vinyl groups strengthen the rigidity of the molecular stucture by creating easier crosslinkage of molecules.

Methoxy and alkoxy groups facilitate cross-linking at low temperatures.

Oils and gums are nonhighly branched or straight-chain polymers whose viscosity increases with the degree of polycondensation.

Styrenics

Polystyrene. Polystyrene has the following formula:

Polystyrene is rigid with excellent dimensional stability, has good chemical resistance to aqueous solutions, and is an extremely clear material.

Impact polystyrene contains polybutadiene added to reduce brittleness. The polybutadiene is usually dispersed as a discrete phase in a continuous polystyrene matrix. Polystyrene can be grafted onto rubber particles, which assures good adhesion between the phases.

Acrylonitrile–Butadiene–Styrene (ABS) Copolymers. This basic three-monomer system can be tailored to yield resins with a variety of properties. Acrylonitrile contributes heat resistance, high strength, and chemical resistance. Butadiene contributes impact strength, toughness, and retention of low-temperature properties. Styrene contributes gloss, processibility, and rigidity. ABS polymers are composed of discrete polybutadiene particles grafted with the styrene–acrylonitrile copolymer; these are dispersed in the continuous matrix of the copolymer.

Styrene–Acrylonitrile (SAN) Copolymers. SAN resins are random, amorphous copolymers whose properties vary with molecular weight and copolymer composition. An increase in molecular weight or in acrylonitrile content generally enhances the physical properties of the copolymer but at some loss in ease of processing and with a slight increase in polymer color.

SAN resins are rigid, hard, transparent thermoplastics which process easily and have good dimensional stability—a combination of properties unique in transparent polymers.

Sulfones

Below are the formulas for three polysulfones.

Polysulfone
$$\begin{bmatrix} CH_3 \\ CH_3 \end{bmatrix}_n$$
Polysulfone
$$\begin{bmatrix} -O & SO_2 & --- \\ SO_2 & --- \\ Poly(ester sulfone) \end{bmatrix}_n$$
Poly(phenyl sulfone)

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The isopropylidene linkage imparts chemical resistance, the ether linkage imparts temperature resistance, and the sulfone linkage imparts impact strength. The brittleness temperature of polysulfones is $-100\,^{\circ}\text{C}$. Polysulfones are clear, strong, nontoxic, and virtually unbreakable. They do not hydrolyze during autoclaving and are resistant to acids, bases, aqueous solutions, aliphatic hydrocarbons, and alcohols.

Thermoplastic Elastomers

Polyolefins. In these thermoplastic elastomers the hard component is a crystalline polyolefin, such as polyethylene or polypropylene, and the soft portion is composed of ethylene–propylene rubber. Attractive forces between the rubber and resin phases serve as labile cross-links. Some contain a chemically cross-linked rubber phase that imparts a higher degree of elasticity.

Styrene–Butadiene–Styrene Block Copolymers. Styrene blocks associate into domains that form hard regions. The midblock, which is normally butadiene, ethylene–butene, or isoprene blocks, forms the soft domains. Polystyrene domains serve as cross-links.

Polyurethanes. The hard portion of polyurethane consists of a chain extender and polyisocyanate. The soft component is composed of polyol segments.

Polyesters. The hard portion consists of copolyester, and the soft portion is composed of polyol segments.

Vinyl

Poly(vinyl chloride) (PVC). Polymerization of vinyl chloride results in the formation of a polymer with the following formula:

$$CH_2 = CHC1 \rightarrow \begin{bmatrix} -CH_2 - CH - \\ C1 \end{bmatrix}_n$$

When blended with phthalate ester plasticizers, PVC becomes soft and pliable.

Its key properties are good resistance to oils and a very low permeability to most gases.

Poly(vinyl acetate). Poly(vinyl acetate) has the following formula:

Poly(vinyl acetate) is used in latex water paints because of its weathering, quick-drying, recoatability, and self-priming properties. It is also used in hot-melt and solution adhesives.

Poly(vinyl alcohol). Poly(vinyl alcohol) has the following formula:

$$\begin{bmatrix} -CH_2 - CH - \\ 0H \end{bmatrix}_n$$

It is used in adhesives, paper coating and sizing, and textile warp size and finishing applications.

Poly(vinyl butyral). Poly(vinyl butyral) is prepared according to the following reaction:

$$\begin{bmatrix} -\operatorname{CH}_2 - \operatorname{CH} - \\ \operatorname{OH} \end{bmatrix}_n + \operatorname{CH}_3 \operatorname{CH}_2 \operatorname{CH}_2 \operatorname{CHO} \rightarrow \begin{bmatrix} -\operatorname{CH}_2 - \operatorname{CH} - \operatorname{CH}_2 - \operatorname{CH} - \\ \operatorname{O} - \operatorname{CH} - \operatorname{O} \\ \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_3 \end{bmatrix}_n$$

Its key characteristics are its excellent optical and adhesive properties. It is used as the interlayer film for safety glass.

Poly(vinylidene chloride). Poly(vinylidene chloride) is prepared according to the following reaction:

$$CH_2$$
= CCl_2 + CH_2 = $CHCl$ \rightarrow [$-CH_2$ - CCl_2 - CH_2 - $CHCl$ -]_n

Random copolymer

Urea Formaldehyde

The reaction of urea with formaldehyde yields the following products, which are used as monomers in the preparation of urea formaldehyde resin.

$$H_2N$$
— CO — NH_2 + H_2CO \rightarrow H_2N — CO — NH — CH_2OH
+ $HOCH_2$ — NH — CO — NH — CH_2OH

The reaction conditions can be varied so that only one of these monomers is formed. 1-Hydroxymethylurea and 1,3-bis(hydroxymethyl)urea condense in the presence of an acid catalyst to produce urea formaldehyde resins. A wide variety of resins can be obtained by careful selection of the pH, reaction temperature, reactant ratio, amino monomer, and degree of polymerization. If the reaction is carried far enough, an infusible polymer network is produced.

Liquid coating resins are prepared by reacting methanol or butanol with the initial hydroxymethylureas. Ether exchange reactions between the amino resin and the reactive sites on the polymer produce a cross-linked film.

	Acetal								
Properties	Homopolymer	Copolymer	20% glass- reinforced homopolymer	25% glass- reinforced copolymer	21% poly(tetrafluoroethylene)- filled homopolymer				
Physical Melting temperature, °C	175	175	101	175	101				
Crystalline Amorphous	175	175	181	175	181				
Specific gravity Water absorption (24 h), % Dielectric strength, KV·mm ⁻¹	1.42 0.25–0.40 19.7	1.41 0.22 19.7	1.56 0.25 19.3	1.61 0.29 22.8	1.54 0.20 15.7				
Electrical Volume (dc) resistivity,									
ohm-cm	1015	1015	5×10 ¹⁴		3×10^{16}				
Dielectric constant (60 Hz) Dielectric constant (10 ⁶ Hz) Dissipation (power) factor (60 Hz)	3.7 3.7	3.7 3.7	3.9 3.9		3.1 3.1				
Dissipation factor (10 ⁶ Hz)	0.005	0.005	0.005		0.005				
Mechanical Compressive modulus, 10³ lb⋅in⁻²	670	450							

Compressive strength, rupture	I	1 1			
or 1% yield, 10^3 lb·in ⁻²	5.29	16 (10%	18 (10%	17 (10%	13 (10%
		yield)	yield)	yield)	yield)
Elongation at break, %	25–75	40–75	7	3	15–22
Flexural modulus at 23 °C,					
10^3 lb·in ²	380-430	375	730	1100	340-350
Flexural strength, rupture or					
yield, $10^3 \mathrm{lb \cdot in^{-2}}$	14	13	15	28	
Hardness, Rockwell (or Shore)	M94	M78	M90	M79	M78
Impact strength (Izod) at 23 °C,					
$J \cdot m^{-1}$	69–123	53-80	43	96	37–64
Tensile modulus, 10 ³ lb⋅in ⁻²	520	410	1000	1250	
Tensile strength at break,					
$10^{3}\mathrm{lb}\cdot\mathrm{in}^{-2}$	10	10	8.5	18.5	7.6
Tensile yield strength,					
$10^3\mathrm{lb}\cdot\mathrm{in}^{-2}$	9.5–12	8.5			6.9–7.6
Thermal					
Burning rate, mm · min ⁻¹	27.9				
Coefficient of linear thermal					
expansion, 10^{-6} °C	100	85	36-81		75
Deflection temperature					
under flexural load					
$(264 \text{lb} \cdot \text{in}^{-2}), ^{\circ}\text{C}$	124	110	157	163	100
Maximum recommended					
service temperature, °C	84				
Specific heat, $\operatorname{cal} \cdot \operatorname{g}^{-1}$	0.35				
Thermal conductivity,					
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.23	0.23			

	Acrylic					Alloy	
						Aorulio	Acrylonitrile– butadiene– styrene-
Properties	Poly(methyl methacrylate)	Cast sheet	Impact- modified	Heat- resistant	Alkyd, molded	Acrylic poly(vinyl chloride) alloy	poly(vinyl chloride) alloy
Physical							
Melting temperature, °C							
Crystalline	90-105	90–105	80–100	100–125		105	
Amorphous							
Specific gravity	1.17-1.20	1.18-1.20	1.11–1.18	1.16–1.19	2.22-2.24		
Water absorption (24h), %	0.1-0.4	0.2-0.4	0.2-0.8	0.2-0.3		0.06	
Dielectric strength, KV·mm ⁻¹	15.7–19.9	17.7–21.7	15.0–19.9	15.7–19.9		>15.7	19.7
Electrical							
Volume (dc) resistivity,							
ohm-cm	$> 10^{14}$	$>10^{14}$					
Dielectric constant (60 Hz)	3.3-4.5	3.5-4.5			3.8-5.0		
Dielectric constant (10 ⁶ Hz)		3.0-3.5			3.6-4.7		
Dissipation (power) factor							
(60 Hz)		0.04-0.06			0.012-0.026		
Dissipation factor (10 ⁶ Hz)		0.02-0.03			0.01-0.016		
Mechanical							
Compressive modulus,							
10^4 lb·in ⁻²	370-460	390–475	240-370	350-460		330-400	

Compressive strength, rupture		1					
or 1% yield, 10 ³ lb·in ⁻²	12-18	11–19	4–14	17	16–20	8.4	
Elongation at break, %	2-10	2–7	20–70	3–5		100	
Flexural modulus at 23°C,							
10 ³ lb • in ⁻²	420-460	390–475	200-380	460-500		330-400	340
Flexural strength, rupture or							
yield, 10 ³ lb⋅in ⁻²	13-19	12–17	7–13	12-16		10.7	9.6
Hardness, Rockwell (or Shore)	M85-M105	M80-M100	R105-R120	M95-M105	E76	R99-R105	R100
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	16–27	16–21	43-133	16–21	27-240	800	560
Tensile modulus, 10 ³ lb⋅in ⁻²	380-450	350-450	200-400	350-460		330-335	330
Tensile strength at break,							
10^{3} lb·in ⁻²	7–11	8-11	5–9	10	4.5–6.5	6.5	5.8
Tensile yield strength,							
10^3 lb·in ⁻²					10–13		
Thermal							
Burning rate, mm∙min ⁻¹		0.5-2.2			Self-		
					extinguishing		
Coefficient of linear thermal							
expansion, 10^{-6} °C	50-90	50-90	50-80	50-60	40-55		46
Deflection temperature under							
flexural load (264 lb·in ⁻²),	74–99	71-102	74–95	88-104	177-204	71	
°C							
Maximum recommended							
service temperature, °C		60–71			220		
Specific heat, cal·g ⁻¹	0.36	0.35					
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.17-0.25	0.17-0.25	0.17-0.21	0.19			

TABLE 10.2 Properties of Commercial Plastics (continued)

	Alloy	Allyl			Cellulosic			
	Polycarbonate acrylonitrile-	Allyl-diglycol-	Diallyl phth	Cellulose acetate		Cellulose- acetate- butyrate resin		
Properties	butadiene– styrene alloy	carbonate polymer	Glass-filled	Mineral-filled	Sheet	Molding	Sheet	
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical Compressive modulus, 103 lb·in-2	150 1.12–1.20 0.21–0.24 17.7	Thermoset 1.3–1.4 0.2 15.0	Thermoset 1.7–2.0 0.12–0.35 15.7–17.7	Thermoset 1.65–1.85 0.2–0.5 15.7–17.7	230 1.27-1.34 2-7 11-24 10 ¹⁰ -10 ¹³ 3.4-7.4 3.2-7.0 0.01-0.06 0.01-0.06	230 1.29–1.34 1.7–6.5 9–24 10 ¹⁰ –10 ¹³ 3.5–7.5 3.2–7.0 0.01–0.06 0.01–0.10	140 1.15–1.22 0.9–2.2 9–18 10 ¹⁰ –10 ¹² 3.7–4.3 3.3–3.8 0.01–0.04 0.01–0.04	

Compressive strength,	1						
rupture or 1% yield,							
10^3 lb·in ⁻²	11	21–23	25–35	20–32	22–33	25–36	
Elongation at break, %	10-15		3–5	3–5	17-40	6–40	50-100
Flexural modulus at 23 °C,							
10^3 lb·in ⁻²	300-400	250–330	1 200-1 500	1000-1400			740–1 300
Flexural strength, rupture or							
yield, 10^3 lb·in ⁻²	13.0-13.7	6–13	9–20	8.5–11	6–10	2–16	4–9
Hardness, Rockwell (or							
Shore)	R117	M95-M100	E80-E87	E61	R85-R120	R100-R123	R50-R95
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	560	11–21	21-800	16–43	107-454	53–214	133–288
Tensile modulus, 10 ³ lb⋅in ⁻²	370–380	300	1400-2200	1 200-2 200			200–250
Tensile strength at break,							
10^3 lb·in ⁻²	7.0–7.3	5–6	6–11	5–8	4.5-8.0	1.9–9.0	2.6-6.9
Tensile yield strength,							
10^3 lb·in ⁻²	8.5				2.2–7.4	4.1–7.6	
Thermal							
Burning rate, mm⋅min ⁻¹						1.3-3.8	1.3-3.8
Coefficient of linear thermal							
expansion, 10 ⁻⁶ °C	63–67	5.4-9.6	0.68-2.4	2.8	100-150	80-180	110-170
Deflection temperature							
under flexural load							
(264 lb⋅in ⁻²), °C	104-116	60-88	165-288+	160–288	44–91	51–98	49–58
Maximum recommended							
service temperature, °C							
Specific heat, cal • g ⁻¹					0.3-0.4	0.3-0.42	0.3-0.4
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.25-0.38	0.20-0.21	0.21-0.63	0.30–1.04	0.17-0.34	0.17-0.34	0.17-0.34

TABLE 10.2 Properties of Commercial Plastics (continued)

		Cellu	ılosic			Epoxy	
	Cellulose- acetate-	Cellulose- acetate-				Bispl	nenol
Properties	butyrate resin, molding	propionate resin, molding	Ethyl cellulose	Cellulose nitrate	Chlorinated polyether	Glass-fiber- reinforced	Mineral- filled
Physical							
Melting temperature, °C							
Crystalline Amorphous	140	190	135		125	Thermoset	Thermoset
Specific gravity	1.15-1.22	1.17-1.24	1.09-1.17	1.35-1.40	1.4	1.6-2.0	1.6-2.1
Water absorption (24h), %	0.9-2.2	1.2-2.8	0.8-1.8			0.04-0.20	0.03-0.20
Dielectric strength, kV·mm ⁻¹	9–13	12-17.7	13.8–19.7			9.8–15.7	9.8–15.7
Electrical							
Volume (dc) resistivity,							
ohm-cm	1010-1012			10^{10}			
Dielectric constant (60 Hz)	3.5-6.4			7.0–7.5			
Dielectric constant (10 ⁶ Hz)	3.2-6.2		3.01	6.6			
Dissipation (power) factor							
(60 Hz)	0.01-0.04						
Dissipation factor (10 ⁶ Hz)	0.01-0.04						
Mechanical							
Compressive modulus,							
10^3 lb·in ⁻²						3000	

Compressive strength, rupture							
or 1% yield, 10^3 lb·in ⁻²	2.1–7.5	2.4–7.0		2.1–8.0		18000-40000	18000-40000
Elongation at break, %	40–88	29–100	5–40	40–45	600–800	4	
Flexural modulus at							
23 °C, 10 ³ lb·in ⁻²	90–300	120–350				2–4.5	
Flexural strength, rupture or					_		
yield, 10 ³ lb⋅in ⁻²	1.8–9.3	2.9–11.4	4–12	9–11	5	8–30	6–18
Hardness, Rockwell (or Shore)	R31–R116	R10-R122	R50-R115	R95–R115	R100	M100-M112	M100-M112
Impact strength (Izod) at							
23°C, J·m ⁻¹	53–582	27 to no break	21	267–374	21	16–533	16–22
Tensile modulus, 10 ³ lb·in ⁻²	50–200	60–215		190–220		3	
Tensile strength at break,	2	20.70			45.40		
10 ³ lb•in ⁻²	2.6–6.9	2.0–7.8	2–8	7–8	1.5–1.8	5–20	4–10
Tensile yield strength,							
10 ³ lb⋅in ⁻²							
Thermal							
Burning rate, mm⋅min ⁻¹	1.3–3.8				Self-		
					extinguishing		
Coefficient of linear thermal							
expansion, 10 ^{−6} °C	110–170	110–170	100-200	80–120	6.6	11–50	20–60
Deflection temperature							
under flexural load							
(264 lb•in ⁻²), °C	44–94	44–109	45–88	60–71	185	107–260	107–260
Maximum recommended							
service temperature, °C					255		
Specific heat, cal·g ⁻¹	0.3-0.4			0.31-0.41			
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.17-0.30	0.17-0.30	0.16-0.30	0.23		0.17-0.42	0.17–1.48

TABLE 10.2 Properties of Commercial Plastics (continued)

		Epoxy			Fluorocarbon				
	Cast	Casting resin		Poly(tetrafl	uoroethylene)	Poly(chloro-			
D C		1	Novolac resin	-	Glass-fiber-	trifluoro-			
Properties Perfluoroalkoxy	Unfilled	Flexible	Mineral-filled	Granular	reinforced	ethylene)			
Physical Melting temperature, °C									
Crystalline	Thermoset	Thermoset	Thermoset	327	327	220	310		
Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹	1.11–1.40 0.08–0.15 11.8–19.7	1.05–1.35 0.27–0.50 9.3–15.8	1.7–2.1 0.05–0.2 11.8–13.8	2.14–2.20 0.01 18.9	2.2–2.3	2.1–2.2 0.03 19.7–23	2.12–2.17		
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Diesctric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical Compressive modulus, 103 lb·in-2	10 ¹² –10 ¹⁷ 3.5–5.0 3.5–5.0			10 ¹⁸ 2.1 2.1 0.0002 0.0002		10 ¹⁸ 2.3–2.7 2.3–2.5 0.001 0.005			

Compressive strength, rupture							
or 1% yield, 10^3 lb·in ⁻²	15–25	1–14	30	1.7		4.6–7.4	
Elongation at break, %	3–6	20–70	2–4	200-400	200–300	80–250	300
Flexural modulus at 23 °C,							
10^3 lb·in ⁻²			2000	80	235	120	
Flexural strength, rupture or					_		
yield, 10^{-3} lb·in ⁻²	13–21	1–13	16–20		2	7.4–9.3	
Hardness, Rockwell (or Shore)	M80-M110			(D50-D55)	(D60-D70)	R75–R95	(D64)
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	10.7–53	187–267	21	160	144	133–160	No break
Tensile modulus, 10 ³ lb·in ⁻²	350	1–350		58–80		150–300	
Tensile strength at break,		2 10	< 10	2 - 7			
10^3 lb·in ⁻²	4–13	2–10	6–12	2–5	2–2.7	4.5–6	4–4.3
Tensile yield strength,			20				
10^3 lb·in ⁻²			30				
Thermal							
Burning rate, mm⋅min ⁻¹				Self-	Self-	Self-	
				extinguishing	extinguishing	extinguishing	
Coefficient of linear thermal							
expansion, 10 ^{−6} °C	45–65	20–100	22–30	100	77–100	70	
Deflection temperature under							
flexural load (264 lb·in ⁻²),	46–288	23–121	149–260	121		126	74 (66 lb • in ⁻²
°C				$(66\mathrm{lb}\cdot\mathrm{in}^{-2})$		$(66 \mathrm{lb} \cdot \mathrm{in}^{-2})$	
Maximum recommended				2.00		200	
service temperature, °C				260		200	
Specific heat, cal·g ⁻¹				0.25		0.22	
Thermal conductivity,	0.17.0.21			0.25	0.24.0.40	0.10.022	0.25
W⋅m ⁻¹ ⋅K ⁻¹	0.17–0.21			0.25	0.34-0.40	0.19-0.22	0.25

TABLE 10.2 Properties of Commercial Plastics (continued)

		Fluorocarbon					
	Fluorinated			fluoroethylene lymer	Ethylene–		
Properties	ethylene- propylene resin	Poly(vinylidene fluoride)	Unfilled	Glass-fiber- reinforced	ethylene copolymer	Cellulose- filled	Glass-fiber- reinforced
Physical							
Melting temperature, °C							
Crystalline	275	156	270	270	245	Thermoset	Thermoset
Amorphous	2.14–2.17	1.75–1.78	1.7	1.8	1.68	1.47–1.52	1.5-2.0
Specific gravity Water absorption (24h), %	<0.01	0.04-0.06	0.03	0.02	0.01	0.1–0.8	0.09–1.3
Dielectric strength, kV·mm ⁻¹	20–24	10	16	17	19	11–16	5–15
Electrical							
Volume (dc) resistivity,							
ohm-cm							
Dielectric constant (60 Hz)	2.1	8–9	2.6		2.6		
Dielectric constant (10 ⁶ Hz)	2.1	8–9	2.6		2.6		
Dissipation (power) factor							
(60 Hz)		High					
Dissipation factor (10 ⁶ Hz)		High					
Mechanical							
Compressive modulus,							
10^3 lb·in ⁻²		120	120	1 200	240		

Compressive strength, rupture			I	1		1	1
or 1% yield, 10^3 lb·in ⁻²	2.2	8.7–10	7.1	10		33–45	20-35
Elongation at break, %	250-330	25-500	100-400	8	200-300	0.6-1.0	0.6
Flexural modulus at							
$23 ^{\circ}\text{C}, 10^{3} \text{lb} \cdot \text{in}^{-2}$	80–95	200	200	950	240	1100	
Flexural strength, rupture or							
yield, $10^3 \mathrm{lb} \cdot \mathrm{in}^{-2}$		8.6–11	5.5	10.7	7	9–16	14–23
Hardness, Rockwell (or Shore)	(D60-D65)	(D80)	R50 (D75)	R74	R95	M115-M125	M115
Impact strength (Izod) at							
23°C, J·m ⁻¹	No break	192–214	No break	480	No break	11–21	32–961
Tensile modulus, 10 ³ lb⋅in ⁻²	50	120	120	1 200	240	1.1–1.4	1.6–2.4
Tensile strength at break, 10 ³ lb·in ⁻²	2.7–3.1	5.5–7.4	6.5	12	7	5–13	5-10.5
Tensile yield strength,	2.7-3.1	3.3-7.4	0.5	12	/	3-13	5-10.5
10 ³ lh·in ⁻²							
10 10 m							
Thermal	NT 4	NT 4	NT 4	NT 4	NT 4	Self-	Self-
Burning rate, mm⋅min ⁻¹	Not combustible	Not	Not combustible	Not combustible	Not combustible		
Coefficient of linear thermal	combustible	combustible	combustible	combustible	combustible	extinguishing	extinguishing
expansion, 10^{-6} °C	83–105	85	59	10–32	80	40–45	15–28
Deflection temperature	65–105	0.5	39	10-32	80	40-43	13-26
under flexural load							
(264lb·in ⁻²), °C	70	80-90	71	210	77	177–199	190-204
(======================================	(66lb·in ⁻²)		, -				
Maximum recommended	,						
service temperature, °C	205	150				210	
Specific heat, cal·g ⁻¹	0.28						
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.25	0.19-0.24	0.24		0.16	0.27-0.41	0.41-0.49
		ļ	1			1	L

TABLE 10.2 Properties of Commercial Plastics (*continued*)

	Melamine phenolic, woodflour- and				Phenolic		
Properties	cellulose- filled	cellulose-	Unfilled	Woodflour- filled	Glass-fiber- reinforced	Cellulose- filled	Mineral- filled
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹	Thermoset 1.5–1.7 0.3–0.65 8.7–12.8	95 1.15 0.28 8.7–9.5	Thermoset 1.24–1.32 0.1–0.36 9.8–15.8	Thermoset 1.37–1.46 0.3–1.2 10.2–15.8	Thermoset 1.69–2.0 0.03–1.2 5.5–15.8	Thermoset 1.38–1.42 0.5–0.9 11.8–15	Thermoset 1.42–1.84 0.1–0.3 7.9–13.8
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical Compressive modulus, 103 lb·in-2		1.9×10 ¹⁵	$ \begin{array}{c} 1 \times 10^{12} \\ $				

Compressive strength, rupture	l				1		
or 1% yield, 10^3 lb·in ⁻²	26–30	12	18-32	25–31	26-70	22-31	22.5-34.6
Elongation at break, %	0.4-0.8	3–4	1.5-2.0	0.4-0.8	0.2	1-2	0.1-0.5
Flexural modulus at							
$23^{\circ}\text{C}, 10^{3}\text{lb}\cdot\text{in}^{-2}$	1000-1200	500-590	700-1500	1000-1200	2000-33000	900-1300	1000-2000
Flexural strength, rupture or							
yield, 10^3 lb·in ⁻²	8–10	14	11–17	7–14	15–60	5.5–11	11–14
Hardness, Rockwell (or Shore)	E95-E100	M72-M76	M93-M120	M100-M115	E54-E101	M95-M115	E88
Impact strength (Izod) at							
23 °C, J ⋅ m ⁻¹	11–21	80–256	13–21	11–32	27–960	21–59	14–19
Tensile modulus, 10 ³ lb⋅in ⁻²	800–1700	510–580	700–1 500	800–1700	1900–3300		2400
Tensile strength at break,					7.10	25.65	6.07
$10^3 \text{lb} \cdot \text{in}^{-2}$	6–8	9	6–9	5–9	7–18	3.5–6.5	6–9.7
Tensile yield strength, 10 ³ lb•in ⁻²			12–15				
			12–15				
Thermal							
Burning rate, mm⋅min ⁻¹			Self-				
Coefficient of linear thermal			extinguishing				
expansion, 10^{-6} °C	10-40	66	68	30–45	8–21	20-31	19–26
Deflection temperature	10-40	00	06	30-43	0-21	20-31	19–20
under flexural load							
(264 lb · in -2), °C	140–154	73	74–80	149–188	177–316	149–177	320-246
Maximum recommended	110 151	73	71 00	117 100	177 510	110 177	320 210
service temperature, °C							
Specific heat, cal·g ⁻¹							
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.17-0.30	0.26	0.15	0.17-0.34	0.34-0.59	0.25-0.38	0.42-0.57

	Polyamide								
	Nylon 6				Nyl	on 6/6			
Properties	Molding and extrusion	30–35% glass- fiber- reinforced	High-impact copolymer	Molding	33% glass- fiber- reinforced	Molybdenum disulfide- filled	Nylon 6/6- nylon 6 copolymer		
Physical									
Melting temperature, °C									
Crystalline	216	216	216	265	265	265	240		
Amorphous									
Specific gravity	1.12–1.14	1.35–1.42	1.08-1.17	1.13–1.15	1.38	1.15–1.17	1.08-1.14		
Water absorption (24h), %	2.9	1.2	1.3–1.5	1.0-1.3	1.0	0.8-1.1	1.5-2.0		
Dielectric strength, kV⋅mm ⁻¹	15.8	15.8	22	24		14	15.8		
Electrical									
Volume (dc) resistivity,									
ohm-cm	10^{12}			1012-1015			10^{10}		
Dielectric constant (60 Hz)	9.8			4.0			16		
Dielectric constant (10 ⁶ Hz)	3.7			3.6			4		
Dissipation (power) factor									
(60 Hz)	0.14			0.01-0.02			0.4		
Dissipation factor (10 ⁶ Hz)	0.12			0.02-0.03			0.1		
Mechanical									
Compressive modulus, 10 ³ lb • in ⁻²	250								

Compressive strength, rupture					I	l I	
or 1% yield, 10^3 lb·in ⁻²	13-16	19		15 (yield)	24.9	12.5	
Elongation at break, %	30-100	3–6	150-270	60	3	15	40
Flexural modulus at 23 °C,							
10^3 lb·in ⁻²	390	1500	110-320	420	1300	450	150-410
Flexural strength, rupture or							
yield, 10 ³ lb⋅in ⁻²	14	33	5-12	17	41	17	
Hardness, Rockwell (or Shore)	R119	M101	R81-R110	R120	M100	R119	R119
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	32–53	160	96 to no	43–53	117	240	37
			break				
Tensile modulus, 10 ³ lb⋅in ⁻²	380	1 450				550	150-410
Tensile strength at break,							
10^3 lb·in ⁻²	11.8	25	7.5–11	12	28	13.7	7.4–12.4
Tensile yield strength,							
10^3 lb·in ⁻²	8			8			
Thermal							
Burning rate, mm·min ⁻¹	Self-						
	extinguishing						
Coefficient of linear thermal							
expansion, 10^{-6} °C	80–90	20–30	30-40	80	15–20	54	
Deflection temperature							
under flexural load							
(264 lb • in ⁻²), °C	68–85	210	45–54	75	249	127	77
Maximum recommended							
service temperature, °C	107			135			
Specific heat, cal·g ⁻¹	0.4			0.4			
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.24	0.24		0.24	0.22		
		-	+				

		Polyamide							
		Nylon 6/12							
Properties	Nylon 6/9, molding and extrusion	Molding	30–35% glass-fiber- reinforced	Nylon 11, molding and extrusion	Nylon 12, molding and extrusion	Aromatic nylon (aramid), molded and unfilled	Poly(amide- imide), unfilled		
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹	205 1.08–1.10 0.5 24	217 1.06–1.08 0.4 16	217 1.31–1.38 0.2 21	194 1.03–1.05 0.3 17	179 1.01–1.02 0.25 18	275 1.30 0.6 31	275 1.40 0.28 24		
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Diescric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz)		10 ¹⁵ 4.0 3.5 0.02 0.02			10 ¹⁴ 3.8 3.0 0.07 0.04				
Mechanical Compressive modulus, 10^3 lb·in ⁻²				180		290	413		

Compressive strength, rupture			I			l	1
or 1% yield, 10 ³ lb•in ⁻²		2.4			7.5	30	40
Elongation at break, %	1125	150	4	300	300	5	12-18
Flexural modulus at							
23 °C, 10 ³ lb·in ⁻²	290	290	1 120	150	165	640	664
Flexural strength, rupture or yield,							
10 ³ lb•in ⁻²					1.5	25.8	30
Hardness, Rockwell (or Shore)	R111	R114	E40-E50	R108	R106-R109	E90	E78
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	59	53	139	96	107–300	75	133
Tensile modulus, 10 ³ lb⋅in ⁻²	275	290	1 200	185	180		730
Tensile strength at break,							
10^3 lb·in ⁻²	8.5	8.8	24	8	8–9	17.5	26.9
Tensile yield strength,							
10 ³ lb•in ⁻²		8.8					
Thermal							
Burning rate, mm⋅min ⁻¹				Self-			
				extinguishing			
Coefficient of linear thermal				77 100	(T. 100	40	26
expansion, 10^{-6} °C		90		55–100	67–100	40	36
Deflection temperature							
under flexural load	57–60	82	02 210	54	54	260	274
(264 lb·in ⁻²), °C Maximum recommended	37-60	82	93–218	34	34	200	274
				100–120			260
service temperature, °C Specific heat, cal•g ⁻¹		0.4		0.58			200
Thermal conductivity,		0.4		0.56			
W·m ⁻¹ ·K ⁻¹		0.22		0.34	0.22	0.22	0.25
** 111 1X		0.22		0.54	0.22	0.22	0.23

TABLE 10.2 Properties of Commercial Plastics (*continued*)

		Polycar	rbonate	Thermoplastic polyester				
	Doly/owyl			Poly(butylene terephthalate)		Poly(ethylene terephthalate)		
Properties	Poly(aryl ether), unfilled	Low viscosity	30% glass-fiber- reinforced	Unfilled	30% glass-fiber- reinforced	Unfilled	30% glass-fiber- reinforced	
Physical								
Melting temperature, °C Crystalline				232–267	232–267	245	245	
Amorphous	160	140	150					
Specific gravity	1.14	1.2	1.4	1.31-1.38	1.52	1.34-1.39	1.27	
Water absorption (24h), %	0.25	0.15	0.14	0.08-0.09	0.06-0.08	0.1-0.2	0.05	
Dielectric strength, kV⋅mm ⁻¹	17	15	19	16–22	18–22		22	
Electrical								
Volume (dc) resistivity,								
ohm-cm		2×10^{16}	$> 10^{16}$		10^{16}	10^{16}		
Dielectric constant (60 Hz)		3.17	3.35					
Dielectric constant (10 ⁶ Hz)		2.96	3.31			3.25		
Dissipation (power) factor								
(60 Hz)		0.0009	0.011					
Dissipation factor (10 ⁶ Hz)		0.010	0.007					
Mechanical								
Compressive modulus,								
10^{3} lb • in ⁻²		350	1300					

Compressive strength, rupture				l ı		1 1	
or 1% yield, 10^3 lb·in ⁻²		12.5	18	8.6–14.5	18-23.5	11-15	25
Elongation at break, %	80	110	3–5	50-300	2–4	50-300	3
Flexural modulus at							
$23^{\circ}\text{C}, 10^{3}\text{lb}\cdot\text{in}^{-2}$	300	340	1 100	330–400	1 100-1 200	35–450	1440
Flexural strength, rupture or							
yield, 10^3 lb·in ⁻²	11	13.5	23	12–16.7	26–29	14–18	33.5
Hardness, Rockwell (or Shore)	R117	M70	M92	M68-M78	M90	M94-M101	M100
Impact strength (Izod) at							
23°C, J·m ⁻¹	427	14	107	43–53	69–85	13–32	101
Tensile modulus, 10 ³ lb⋅in ⁻²	320	345	1250	280	1 300	400–600	1 440
Tensile strength at break, 10 ³ lb·in ⁻²	7.5	9.5	19	8.2	17–19	0.5.10.5	23
Tensile yield strength,	7.5	9.5	19	8.2	17-19	8.5–10.5	23
$10^3 \mathrm{lb} \cdot \mathrm{in}^{-2}$		9.0					
		9.0					
Thermal		G 16	0.10				
Burning rate, mm⋅min ⁻¹		Self-	Self-				
Coefficient of linear thermal		extinguishing	extinguishing				
expansion, 10^{-6} °C	65	68	22	60–95	25	65	29
Deflection temperature	03	00	22	00-23	23	03	2)
under flexural load							
(264 lb • in ⁻²), °C	149	138-145	146	50-85	220	38–41	224
Maximum recommended							
service temperature, °C		143					
Specific heat, cal·g ⁻¹		0.3				0.27	
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.30	0.20	0.22	0.18-0.30	0.30	0.15	

TABLE 10.2 Properties of Commercial Plastics (continued)

	Thermoplastic polyester Aromatic polyester			Thermosetting and alkyd polyester					
			Unsaturated j	polyester	Alkyd molding compounds				
Properties	Extrusion- transparent	Injection molding	Styrene-maleic acid copolymer, low-shrink	Butadiene- maleic acid copolymer	Putty, mineral-filled	Glass-fiber- reinforced	Polyimide, unfilled		
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹	81	1.39 0.01 14	Thermoset	Thermoset	Thermoset	Thermoset	310–365 1.36–1.43 0.24 22		
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dislectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz)							>10 ¹⁶ 3-4		
Mechanical Compressive modulus, 10³ lb·in⁻² Compressive strength, rupture or 1% yield, 10³ lb·in⁻²		10	15–30	14–30	2000–3000 12–38	15–36	30–40		

Elongation at break. %	225	7–10	3–5				8-10
Flexural modulus at $23 ^{\circ}\text{C}$, $10^{3} \text{lb} \cdot \text{in}^{-2}$	290	700	1000-2500		2000	2000	450–500
Flexural strength, rupture or	290	700	1000-2300		2000	2000	430–300
yield, 10^3 lb·in ⁻²	10.6	12	9–35	16–24	6–17	8.5–26	19–28.8
Hardness, Rockwell (or Shore)	R105		40–70 (Barcol)	50–60 (Barcol)	E98	E95	E52–E99
Impact strength (Izod) at				<u> </u>			
23 °C, J⋅m ⁻¹	101		133-800	214–694	16-27	27-854	80
Tensile modulus, 10 ³ lb⋅in ⁻²		300	1 000-2 500	1500-2500	500-3000		300
Tensile strength at break,							
10^3 lb·in ⁻²	6	11	4.5–20	5–10	3–9	4–9.5	10.5–17.1
Tensile yield strength,							
10^3 lb·in ⁻²	7						12.5
Thermal							
Burning rate, mm·min ⁻¹							
Coefficient of linear thermal							
expansion, 10^{-6} °C		29	6–30		20–50	15–33	45–56
Deflection temperature							
under flexural load	63	282	190–260	160–177	177–260	204–260	277–360
(264 lb⋅in ⁻²), °C Maximum recommended	03	282	190-200	100-177	177-200	204-200	277-300
service temperature, °C							
Specific heat, cal•g ⁻¹							0.27
Thermal conductivity,							0.27
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$		0.29		0.76-0.93	0.51-0.89	0.6-0.89	0.10-0.11

		Polyolefin								
			Polyethylene							
Properties	Poly(methyl pentene), unfilled	Low-density	Medium-density	High-density	Ultra high- molecular- weight	Glass-fiber- reinforced, high-density	Ethylene– vinyl acetate copolymer			
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24 h), % Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (10 ⁶ Hz) Dissipation (power) factor (60 Hz) Dissipation factor (10 ⁶ Hz) Mechanical Compressive modulus,	230–240 0.84 0.01	95-130 0.910-0.925 < 0.01 18-39 >10 ¹⁵ 2.3 2.3 < 0.0005 < 0.0005	120–140 0.926–0.94 < 0.01 18–39 > 10 ¹⁵ 2.3 2.3 < 0.0005 < 0.0005	120-140 0.941-0.965 <0.01 18-39 <10 ¹⁵ 2.3 2.3 <0.0005 <0.0005	125–135 0.94 <0.01 28	120–140 1.28 0.02 20	65–90 0.92–0.95 0.05–0.13 24–30			
10^3 lb·in ⁻²	114–171									

Compressive strength, rupture		1 1		I	I	l	I
or 1% yield, 10 ³ lb·in ⁻²	5-6.6			2.7–3.6		7	
Elongation at break, %	10-50	90-800	50-600	20-130	450–525	1.5	550-900
Flexural modulus at							
$23^{\circ}\text{C}, 10^{3}\text{lb}\cdot\text{in}^{-2}$	110-260	8-60	60-115	100-260	130–140	800	1–20
Flexural strength, rupture or							
yield, 10 ³ lb⋅in ⁻²	4-6.5					11	
Hardness, Rockwell (or Shore)	L67-L74	(D40-D51)	(D50-D60)	R30-R50	R50	R75	
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	16–64	No break	27-854	27–1068	No break	59	No break
Tensile modulus, 10 ³ lb⋅in ⁻²	160–280	14–38	25–55	60–180			20–120
Tensile strength at break,						_	
10 ³ lb • in ^{−2}	3.5–4	0.6–2.3	1.2–3.5	3.1–5.5	5.6	9	1.4–2.8
Tensile yield strength,		00.42	1000		2.1.10		
10^3 lb·in ⁻²		0.8–1.2	1.0–2.2	3–4	3.1–4.0		
Thermal							
Burning rate, mm⋅min ⁻¹		1.0	1.0	1.0			
Coefficient of linear thermal							
expansion, 10^{-6} °C	117	100–220	140–160	110–130	130	48	160–200
Deflection temperature							
under flexural load		22 44	44 40	10.51	12 10	101	
(264 lb⋅in ⁻²), °C	41	32–41	41–49	43–54	43–49	121	34
Maximum recommended	175	70	93	200			
service temperature, °C Specific heat, cal·g ⁻¹	1/5	0.55	0.55	0.46-0.55			
Thermal conductivity,		0.33	0.33	0.40-0.33			
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.17	0.34	0.34-0.42	0.46-0.51		0.46	
W III K	0.17	0.54	0.54-0.42	0.40-0.31		0.40	

TABLE 10.2 Properties of Commercial Plastics (continued)

			Polyolefin					
			Polypropylene				40%	
Properties	Polybutylene extrusion	Homopolymer	Copolymer	Impact copolymer	Polyallomer	Injection molding	glass-fiber- reinforced	
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity,	126 0.91–0.925 0.01–0.02 18	168 0.90–0.91 0.01–0.03 24	160–168 0.89–0.905 0.03 24	0.90 < 0.03 24	120–135 0.90 <0.01 31	290 1.3 < 0.02 15	290 1.6 0.05 18	
ohm-cm Dielectric constant (60 Hz) Dielectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz)		$ \begin{array}{c} 10^{17} \\ 2.2-2.6 \\ 2.2-2.6 \end{array} $ $ < 0.0005 \\ 0.0005-0.002 $	10 ¹⁷ 2.3 2.3 0.0001-0.0005 0.0001-0.002	10 ¹⁷ 2.3 0.0003				
Mechanical Compressive modulus, 10 ³ lb·in ⁻²	31	150–300						

Compressive strength, rupture	1	I	I	1 1	ı	ı	
or 1% yield, 10^3 lb·in ⁻²		5.5-8.0	3.5-8.0			16	21
Elongation at break, %	300-380	100-600	200-700	8–20	400-500	1–2	1
Flexural modulus at							
$23 ^{\circ}\text{C}, 10^{3} \text{lb} \cdot \text{in}^{-2}$	45-50	170–250	130-200	130-190	70-110	550	1700
Flexural strength, rupture or							
yield, 10^3 lb·in ⁻²	2-2.3	6–8	5–7			14	29
Hardness, Rockwell (or Shore)		R80-R102	R50-R96	R40-R90	R50-R85	R123	R123
Impact strength (Izod) at							
23°C, J·m ⁻¹	No break	21–53	53-1068	80–900	91–203	< 27	75
Tensile modulus, 10 ³ lb⋅in ⁻²	30–40	165–225	100–170			480	1 100
Tensile strength at break,							
10^3 lb·in ⁻²	3.8–4.4	4.5–6	4–5.5		3–3.8	9.5	19.5
Tensile yield strength,	1505		2 7 4 2		2 2 4		
10 ³ lb⋅in ⁻²	1.7–2.5	4.5–5.4	3.5–4.3	2.5–3.1	3–3.4		
Thermal							
Burning rate, mm•min ⁻¹ Coefficient of linear thermal							
expansion, 10^{-6} °C	128–150	81–100	68–95	60–90	83–100	49	22
Deflection temperature	120-130	81-100	08-93	00-90	83-100	49	22
under flexural load							
(2641b·in ⁻²), °C	54–60	48–57	45–57	90–105	51–56	135	249
(20+10 III), C	34 00	10 37	73 31	(66 lb·in ⁻²)	31 30	133	247
Maximum recommended				(0010 111)			
service temperature, °C		160	240	140–160			
Specific heat, cal·g ⁻¹		0.44-0.46	0.45-0.50	0.45-0.50			
Thermal conductivity,							
$W \cdot m^{-1} \cdot K^{-1}$	0.22	0.12	0.15-0.17	0.12-0.17	0.09-0.17	0.29	0.29

TABLE 10.2 Properties of Commercial Plastics (continued)

	Polyurethane					Styrenic	
	Castin	ng resin	Thermonlestic	Coot regin	Mineral- and/or	Epoxy molding and	Polystyrene
Properties	Liquid	Unsaturated	Thermoplastic elastomer	Cast resin, flexible	glass-filled	encapsulating compound	Crystal
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical	Thermoset 1.1–1.5 0.02–1.5 12–20 10 ¹¹ –10 ¹⁵ 4.0–7.5	Thermoset 1.05 0.1–0.2	120–160 1.05–1.25 0.7–0.9 13–25 10 ¹¹ –10 ¹³ 5.4–7.6	Thermoset 0.99–1.5 22 10 ¹⁴ –10 ¹⁵ 2.7–4.2	Thermoset 1.8–1.94 8–15	Thermoset 1.84 10	$85-105$ $1.04-1.05$ $0.03-0.10$ 24 $>10^{16}$ 2.5
Compressive modulus, 10 ³ lb·in ⁻²	10–100		4–9				

Compressive strength, rupture or 1% yield, 10 ³ lb·in ⁻²	20	2.6	20	100, 700	10–16	28	11.5–16
Elongation at break, %	100–1000	3–6	100–1100	100–700			1–2
Flexural modulus at 23 °C, 10 ³ lb·in ⁻² Flexural strength, rupture or	10–100	610	10–350		1000-2500		380–450
yield, 10 ³ lb·in ⁻² Hardness, Rockwell (or Shore)	0.7–4.5	19	0.7–9 (A65–D80)	(A15–A65)	9-14 M80-M90	17	8–14 M60–M75
Impact strength (Izod) at 23 °C, J·m ⁻¹	1334 to	21	No break		13–427	16	13–21
Tensile modulus, 10 ³ lb • in ⁻²	10–100		10-350				350–485
Tensile strength at break,							
10 ³ lb⋅in ⁻²	0.175–10	10–11	1.5-8.4	0.35-1.0	4-6.5	6–8	5.3–7.9
Tensile yield strength,							
10^3 lb·in ⁻²							
Thermal					0.70		
Burning rate, mm·min ⁻¹					0–78		
Coefficient of linear thermal expansion, 10^{-6} °C	100-200		100-200	300-800	20-50	30	70–80
Deflection temperature under	100-200		100-200	300-800	20-30	30	70-80
flexural load	Varies over	87–93	Varies over		260	74–100	
(264 lb • in ⁻²), °C	wide range		wide range				
Maximum recommended							
service temperature, °C					371		93
Specific heat, cal·g ⁻¹	0.43		0.43				0.3
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.21		0.07-0.31	0.15-0.31	0.30	0.68	0.09-0.13

TABLE 10.2 Properties of Commercial Plastics (*continued*)

		Styrenic								
	Polystyrene			Acrylonitrile-butadiene-styrene copolymer						
•					Molding					
Properties	Heat- resistant	Extrusion	Heat- resistant	High-impact	Flame- retarded	Platable	20% glass- reinforced			
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), % Dielectric strength, kV·mm ⁻¹	110–125 1.05–1.09 0.03–0.12 20	88–120 1.02–1.06 0.20–0.45 14–20	110–125 1.05–1.08 0.20–0.45 14–20	100–110 1.01–1.04 0.20–0.45 14–20	110–125 1.16–1.21 0.2–0.6 14–20	100–110 1.06–1.07 16–22	1.22			
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (10 ⁶ Hz) Dissipation (power) factor (60 Hz) Dissipation factor (10 ⁶ Hz) Mechanical Compressive modulus, 10 ³ lb · in ⁻²		150–390	190–440	2.4–5.0 2.4–3.8 0.003–0.008 0.007–0.015	130–310					

Compressive strength, rupture		1	1		1		
or 1% yield, 10 ³ lb·in ⁻²	11.5–16	5.2–10	7.2–10	4.5-8	6.5-7.5		14
Elongation at break, %	2-60	20–100	3–20	5-70	5–25		
Flexural modulus at							
23 °C, 10 ³ lb • in ⁻²	340-470	130-420	300–400	250-350	300-400	340–390	710
Flexural strength, rupture or							
yield, 10 ³ lb⋅in ⁻²	8.9–14	4–14	10–13	8-11	9–14	10.5–11.5	15.5
Hardness, Rockwell (or Shore)	L80-L108	R75-R115	R100-R115	R85-R105	R100-R120	R103-R109	M85
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	21–181	133–640	107–347	347-400	160-640	267–283	64
Tensile modulus, 10 ³ lb⋅in ⁻²	320-460	130–380	300–350	230–330	320-400	330–380	740
Tensile strength at break,							
10 ³ lb•in ⁻²	5–7.8	2.5–8.0	6–7.5	4.8–6.3	5–8	6–6.4	11
Tensile yield strength,							
10 ³ lb • in ⁻²			5.5–7	4–5.5	4–6		
Thermal							
Burning rate, mm∙min ⁻¹		1.3		1.3			
Coefficient of linear thermal							
expansion, 10^{-6} °C	60–70	60–130	60–93	95-110	65–95	47–53	21
Deflection temperature							
under flexural load							
(264 lb • in ⁻²), °C	93-120	77–104	104–116	96-102	90-107	96–102	99
		annealed	annealed	annealed	annealed	annealed	
Maximum recommended							
service temperature, °C				110			
Specific heat, cal·g ⁻¹				0.3-0.4			
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$			0.19-0.34				
		-			1		

TABLE 10.2 Properties of Commercial Plastics (*continued*)

		Styrenic			Sulfone				
	Styrene-acrylonitrile copolymer			Polysulfon	Polysulfone				
Properties	Unfilled	20% glass-fiber- reinforced	Styrene— butadiene copolymer, high-impact	Unfilled	20% glass-fiber- reinforced	Poly(ether sulfone)	Poly(phenyl sulfone)		
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24h), %	115–125 1.07–1.08 0.2–0.3	115–125 1.22 0.15–0.20	90–110 1.03–1.06 0.05–0.10	200 1.24 0.22	200 1.46 0.23	230 1.37 0.43	220 1.29 1.1–1.3 (saturated)		
Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (10 ⁶ Hz) Dissipation (power) factor (60 Hz) Dissipation factor (10 ⁶ Hz)	16–20	20	18	17 10 ¹⁵ 3.14 3.26 0.004 0.008	3.7 3.7 0.002 0.009	17	(saturated) 16		
Mechanical Compressive modulus, 10^3 lb·in ⁻²	530			370					

Compressive strength, rupture							
of 1% yield, 10 ³ lb • in ⁻²	14–17	19	4–9	13.9	22		
Elongation at break, %	1–4	1–2	13-50	50-100	2	30–80	60
Flexural modulus at							
$23^{\circ}\text{C}, 10^{3}\text{lb}\cdot\text{in}^{-2}$	550	100-1100	280-450	390	1000	375	330
Flexural strength, rupture or							
yield, 10 ³ lb⋅in ⁻²	14–17	20	5.3-9.4	15.4	23	18.7	12.4
Hardness, Rockwell	M80-M90	R122	M10-M68	M69, R120	R123	M88	
(or Shore)							
Impact strength (Izod) at							
23 °C, J⋅m ⁻¹	19–27	53	32-192	64	59	85	640
Tensile modulus, 10 ³ lb⋅in ⁻²	400–560	1 150-1 200	280-465	360	1 200	350	310
Tensile strength at break,							
10^3 lb·in ⁻²	9–12	15.8–18	3.2-4.9		17		
Tensile yield strength,							
10^3 lb·in ⁻²			2.9-4.9	10.2		12.2	10.4
Thermal							
Burning rate, mm⋅min ⁻¹							
Coefficient of linear thermal							
expansion, 10^{-6} °C	36–38	38-40	70-101	52-56	25	55	31
Deflection temperature							
under flexural load							
(264 lb • in ⁻²), °C	88-104	99	74–93	174	182	203	204
Maximum recommended							
service temperature, °C				149			
Specific heat, cal·g ⁻¹							
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.12	0.26-0.28	0.12-0.21	0.12	0.38	0.14-0.19	

TABLE 10.2 Properties of Commercial Plastics (continued)

		Thermoplastic el	astomers		Vinyl		
			Block copolymers of styrene and	Block copolymers of styrene and	Urea	Poly(vinyl chloride) and poly(vinyl acetate)	
Properties	Polyolefin	Polyester	butadiene or styrene and isoprene	ethylene or styrene and butylene	formaldehyde, alpha-cellulose filled	Rigid	Flexible and unfilled
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24 h), % Dielectric strength, kV·mm ⁻¹ Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Dielectric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical	0.88-0.90 0.01 24-26	168–206 1.17–1.25	0.9–1.2 0.19–0.39 16–21	0.9–1.2	Thermoset 1.47–1.52 0.4–0.8 12–16 0.5–5.0 7.7–9.5 6.7–8.0 0.036–0.043 0.025–0.035	75–105 1.30–1.58 0.04–0.4 14–20 10 ¹² –10 ¹⁵ 3.2–4.0 3.0–4.0 0.01–0.02 0.006–0.02	75–105 1.16–1.35 0.15–0.75 12–16 10 ¹¹ –10 ¹⁴ 5.0–9.0 3.0–4.0 0.03–0.05 0.06–0.1
Compressive modulus, $10^3 \mathrm{lb} \cdot \mathrm{in}^{-2}$			3.6–120				

Compressive strength, rupture or 1% yield, 10 ³ lb·in ⁻²	150, 200	250, 450	500 1250	C00, 200	25–45	8–13	0.9–1.7
Elongation at break, %	150–300	350–450	500–1350	600–800	<1	40–80	200–450
Flexural modulus at 23 °C, 10 ³ lb·in ⁻²	1.5–2.0	7–75	4–150	4–100	1 300–1 600	300-500	
Flexural strength, rupture or yield, 10 ³ lb·in ⁻²					10–18	10–16	
Hardness, Rockwell (or Shore) Impact strength (Izod) at	(A65–A92)	(D40-D72)	(A40-A90)	(A50–A90)	M110–M120	(D65–D95)	(A50–A100)
23°C, J·m ⁻¹	No break	208 to no break	No break	No break	13–21	21–1068	Varies over wide range
Tensile modulus, 10 ³ lb·in ⁻² Tensile strength at break,		1.1–2.5	0.8–50		1000-1500	350-600	
10^3 lb·in ⁻²	0.65–2.0	3.7-5.7	0.6-3.0	1–3	5.5–13	6–75	1.5–3.5
Tensile yield strength, 10 ³ lb⋅in ⁻²							
Thermal							
Burning rate, mm⋅min ⁻¹					Self- extinguishing	Self- extinguishing	Slow to self- extinguishing
Coefficient of linear thermal							
expansion, 10 ⁻⁶ °C	130–170		130–137		22–36	50-100	70–250
Deflection temperature under flexural load							
(264 lb • in ⁻²), °C			< 0-49		127–143	60–77	
Maximum recommended					77	70.74	00 105
service temperature, °C Specific heat, cal•g ⁻¹					77 0.6	70–74 0.2–0.28	80–105 0.36–0.5
Thermal conductivity,							
$\mathbf{W} \cdot \mathbf{m}^{-1} \cdot \mathbf{K}^{-1}$	0.19-0.21		0.15		0.30-0.42	0.15-0.21	0.13-0.17

	Vinyl						
	Poly(vinyl chloride) and poly(vinyl acetate)	Poly(vinyl			Chlorinated	Poly(viny)	
Properties	Flexible and filled	chloride), 15% glass-fiber- reinforced	Poly(vinylidene chloride)	Poly(vinyl formal)	poly(vinyl chloride)	Poly(vinyl butyral), flexible	
Physical Melting temperature, °C Crystalline Amorphous Specific gravity Water absorption (24 h), % Dielectric strength, kV·mm ⁻¹	75–105 1.3–1.7 0.5–1.0 9.8–12	75–105 1.54 0.01 24–31	210 1.65–1.72 0.1 16–24	105 1.2–1.4 0.5–3.0 19	110 1.49–1.56 0.02–0.15	49 1.05 1.0–2.0 14	
Electrical Volume (dc) resistivity, ohm-cm Dielectric constant (60 Hz) Diesctric constant (106 Hz) Dissipation (power) factor (60 Hz) Dissipation factor (106 Hz) Mechanical Compressive modulus, 103 lb·in-2			10 ¹⁴ –10 ¹⁶ 4.5–6.0		335–600		

Compressive strength, rupture				1	1	
or 1% yield, 10^3 lb·in ⁻²	1.0-1.8	9	2–2.7		9–22	
Elongation at break, %	200-400	2–3	50-250	5–20	4–65	150-450
Flexural modulus at						
$23 ^{\circ}\text{C}, 10^{3} \text{lb} \cdot \text{in}^{-2}$		750			380–450	
Flexural strength, rupture or						
yield, 10 ³ lb⋅in ⁻²		13.5	4.2–6.2	17–18	14.5–17	
Hardness, Rockwell (or Shore)	(A50-A100)	R118	M50-M65	M85	R117–R122	A10-A100
Impact strength (Izod) at			46.50	42.55		
23 °C, J⋅m ⁻¹	Varies over	53	16–53	43–75	53–299	Varies over
T 1 1 10311 1 -2	wide range	070	50.00	250 600	260 475	wide range
Tensile modulus, 10 ³ lb·in ⁻²		870	50–80	350–600	360–475	
Tensile strength at break, 10 ³ lb·in ⁻²	1–3.5	9.5	3–5	10–12	7.5–9	0.5-3.0
Tensile yield strength,	1-3.3	9.3	3–3	10-12	1.3-9	0.3-3.0
10 ³ lb·in ⁻²						
Thermal						
Burning rate, mm⋅min ⁻¹			Self-			Slow
C (C' ' (C1') 1 1			extinguishing			
Coefficient of linear thermal			100	(4	(0.70	
expansion, 10 ⁻⁶ °C			190	64	68–78	
Deflection temperature under flexural load						
(264 lb • in -2), °C		68	54–71	71–77	94–112	
Maximum recommended		00	J 4- /1	/1-//	74-112	
service temperature, °C			100			
Specific heat, cal·g ⁻¹			0.32			
Thermal conductivity,			0.52			
W•m ⁻¹ •K ⁻¹	0.13-0.17		0.13	0.16	0.14	
,, 111 12	0.13 0.17		0.13	0.10	J.17	

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FORMULAS AND ADVANTAGES OF RUBBERS

Gutta Percha

Gutta percha is a natural polymer of isoprene (3-methyl-1,3-butadiene) in which the configuration around each double bond is *trans*. It is hard and horny and has the following formula:

$$\begin{bmatrix} CH_3 \\ C \\ CH_2 \end{bmatrix}_n$$

Natural Rubber

Natural rubber is a polymer of isoprene in which the configuration around each double bond is cis (or Z):

Its principal advantages are high resilience and good abrasion resistance.

Chlorosulfonated Polyethylene

Chlorosulfonated polyethylene is prepared as follows:

$$[-CH_2-CH_2-]_n + HSO_3CI \rightarrow \begin{bmatrix} -CH_2-CH-\\ SO_3H \end{bmatrix}_n + HCI$$

Cross-linking, which can occur as a result of side reactions, causes an appreciable gel content in the final product.

The polymer can be vulcanized to give a rubber with very good chemical (solvent) resistance, excellent resistance to aging and weathering, and good color retention in sunlight.

Epichlorohydrin

Epichlorohydrin is a product of covulcanization of epichlorohydrin (epoxy) polymers with rubbers, especially *cis*-polybutadiene.

Its advantages include impermeability to air, excellent adhesion to metal, and good resistance to oils, weathering, and low temperature.

Nitrile Rubber (NBR, GRN, Buna N)

Nitrile rubber can be prepared as follows:

Nitrile rubber is also known as nitrile-butadiene rubber (NBR), government rubber nitrile (GRN), and Buna N.

It possesses resistance to oils up to 120°C and excellent abrasion resistance and adhesion to metal.

Polyacrylate

Polyacrylate has the following formula:

$$\begin{bmatrix} -CH_2 - CH - \\ | \\ | \\ | \\ | \\ | \end{bmatrix}_n$$

It possesses oil and heat resistance to 175°C and excellent resistance to ozone.

cis-Polybutadiene Rubber (BR)

cis-Polybutadiene is prepared by polymerization of butadiene by mostly 1,4-addition.

$$CH_2 = CH - CH = CH_2 \rightarrow [-CH_2 - CH = CH - CH_2 -]_n$$

The polybutadiene produced is in the *Z* (or *cis*) configuration.

cis-Polybutadiene has good abrasion resistance, is useful at low temperature, and has excellent adhesion to metal.

Polychloroprene (Neoprene)

Polychloroprene is prepared as follows:

$$\begin{array}{c} \operatorname{CH}_2 = \operatorname{CH} - \operatorname{C} = \operatorname{CH}_2 \to \begin{bmatrix} -\operatorname{CH}_2 - \operatorname{CH} = \operatorname{C}(\operatorname{Cl}) - \operatorname{CH}_2 - \end{bmatrix}_n \\ \operatorname{Cl} \end{array}$$

It has very good weathering characteristics, is resistant to ozone and to oil, and is heat-resistant to 100 °C.

Ethylene-Propylene-Diene Rubber (EPDM)

Ethylene–propylene–diene rubber is polymerized from 60 parts ethylene, 40 parts propylene, and a small amount of nonconjugated diene. The nonconjugated diene permits sulfur vulcanization of the polymer instead of using peroxide.

It is a very lightweight rubber and has very good weathering and electrical properties, excellent adhesion, and excellent ozone resistance.

Polyisobutylene (Butyl Rubber)

Polyisobutylene is prepared as follows:

$$\begin{array}{ccc}
CH_{3} & CH_{3} \\
H_{3}C-C=CH_{2}+CH_{2}=C-CH=CH_{2} \rightarrow \begin{bmatrix}
CH_{3} \\
-C-CH_{2}-\\
CH_{3}
\end{bmatrix} - CH_{2}-C=CH-CH_{2}-\end{bmatrix}$$
98 parts 2 parts

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It possesses excellent ozone resistance, very good weathering and electrical properties, and good heat resistance.

(Z)-Polyisoprene (Synthetic Natural Rubber)

Polymerization of isoprene by 1,4-addition produces polyisoprene that has a cis (or Z) configuration.

$$\begin{bmatrix} H_3C & H \\ C=C & CH_2 - \end{bmatrix}_n$$

Polysulfide Rubbers

Polysulfide rubbers are prepared as follows:

$$Cl-R-Cl+Na-S-S-S-S-Na \rightarrow HS[-R-S-S-S-S-S-]_R-SH$$

where R can be

$$-CH_{2}CH_{2}-, -CH_{2}CH_{2}-O-CH_{2}CH_{2}-,$$

or

$$-CH_{2}CH_{2}-O-CH_{2}-O-CH_{2}CH_{2}-.$$

Polysulfide rubbers possess excellent resistance to weathering and oils and have very good electrical properties.

Poly(vinyl chloride) (PVC)

Poly(vinyl chloride) as previously discussed under "Formulas and Key Properties of Plastic Materials" has the following structures:

$$\begin{bmatrix} -CH_2 - CH - \\ Cl \end{bmatrix}_n$$

PVC polymer plus special plasticizers are used to produce flexible tubing which has good chemical resistance.

Silicone Rubbers

Silicone rubbers are prepared as follows

$$\begin{array}{ccc}
CH_3 & CH_3 \\
CI-Si-CI \xrightarrow{H_2O} & HO-Si-OH \xrightarrow{polymerize} & \begin{bmatrix}
CH_3 \\
-Si-O-\\
CH_3
\end{bmatrix},$$

$$CH_3 & CH_3$$

Other groups may replace the methyl groups.

Silicone rubbers have excellent ozone and weathering resistance, good electrical properties, and good adhesion to metal.

Styrene-Butadiene Rubber (GRS, SBR, Buna S)

Styrene—butadiene rubber is prepared from the free-radical copolymerization of one part by weight of styrene and three parts by weight of 1,3-butadiene. The butadiene is incorporated by both 1,4-addition (80%) and 1,2-addition (20%). The configuration around the double bond of the 1,4-adduct is about 80% *trans*. The product is a random copolymer with these general features:

Styrene-butadiene rubber (SBR) is also known as government rubber styrene (GRS) and Buna S.

Urethane

See Table 10.3.

TABLE 10.3 Properties of Natural and Synthetic Rubbers

	Smarifia	Durometer hardness	Ultimate	Tensile	Service temperature, °C	
Rubber	Specific gravity	(or Shore)	elongation % (23°C)	strength, lb·in ⁻² (23°C)	Minimum	Maximum
Gutta percha (hard rubber)	1.2–1.95	(65–95)	3–8	4000-1 0,000		104
Natural rubber (NR)	0.93	20–100	750-850	3000-4500	-56	82
Chlorosulfonated polyethylene	1.10	50–95	100-500	500-3000	-54	121
Epichlorohydrin	1.27	60–90	100-400	1000-2500	-46	121
Fluoroelastomers	1.4-1.95	60–90	100-350	2000-3000	-40	232
Isobutene-isoprene rubber (IIR) [also known as						
government rubber I(GR-I)]	0.91	(40–70)	750–950	2300-3000		121
Nitrile rubber (butadiene-acrylonitrile rubber) (also						
known as Buna N and NBR)	1.00	30–100	100-600	500-4000	-54	121
Polyacrylate	1.10	40–100	100-400	1000-2200	-18	149
Polybutadiene rubber (BR)	0.93	30–100	100-700	2500-3000	-62	79–100
Polychloroprene (neoprene)	1.23	20–90	800-1000	2000-3500	-54	121
Poly(ethylene-propylene-diene) (EPDM)	0.85	30-100	100-300	1000-3000	-40	149
Polyisobutylene (butyl rubber)	0.92	30-100	100-700	1000-3000	-54	100
Polyisoprene	0.94	20-100	100-750	2000-3000	-54	79–82
Polysulfide (Thiokol ST)	1.34	20-80	100-400	700-1250	-54	82-100
Poly(vinyl chloride) (Koroseal)	1.32	(80-90)		2400-3000		71
Silicone, high-temperature				700-800		316
Silicone	0.98	20–95	50-800	500-1500	-84	232
Styrene-butadiene rubber (SBR) (also known as Buna S)	0.94	40–100	400-600	1600-3700	-60	107
Urethane	0.85	62–95	100-700	1000-8000	-54	100

CHEMICAL RESISTANCE

TABLE 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C

The information in this table is intended to be used only as a general guide. The chemical resistance classifications are E = excellent (30 days of exposure causes no damage), G = good (some damage after 30 days), F = fair (exposure may cause crazing, softening, swelling, or loss of strength), N = not recommended (immediate damage may occur).

							Chemica	ıl					
	Acids, dilute or weak	Acids, strong and concentrated	Alcohols, aliphatic	Aldehydes	Alkalies, concentrated	Esters	Ethers	Glycols	Hydrocarbons, aliphatic	Hydrocarbons, aromatic	Hydrocarbons, halogenated	Ketones	Oxidizing agents, strong
			Polymer	S									
Acetals	F	N	F	N	N	N	N	G	N	N	N	N	N
Acrylics: poly(methyl methacrylate)	G	N	Е		N	N	E	E	G	N	N	N	N
Allyls: diallyl phthalate	G				N				E	G	G	N	
Cellulosics: cellulose-acetate-butyrate and cellulose-acetate- propionate polymers	F	N	N	N	N	N	N	G	F	N	N	N	
Fluorocarbons	E	E	Е	E	Е	Е	Е	Е	E	Е	Е	Е	E
Polyamides	N	N	G	E	Е	G		G	G	F	F	G	N
Polycarbonates	G	N	G	F	N	N	N	G	N	N	N	N	N
Polyesters	G	G	N		N	N	F	G	G	F	F	N	F
Poly(methyl pentene)	E	E	G	G	Е	G	N	E	F	G	N	F	F
Low-density polyethylene	E	E	Е	G	Е	G	N	E	F	F	N	G	F
High-density polyethylene	E	Е	Е	E	Е	G	N	E	G	G	N	G	F
Polybutadiene	G	F	Е							Е	E	Е	

TABLE 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C (*continued*)

						(Chemica	ıl					
	Acids, dilute or weak	Acids, strong and concentrated	Alcohols, aliphatic	Aldehydes	Alkalies, concentrated	Esters	Ethers	Glycols	Hydrocarbons, aliphatic	Hydrocarbons, aromatic	Hydrocarbons, halogenated	Ketones	Oxidizing agents, strong
		Poly	mers (ca	ontinue	d)								
APolypropylene and polyallomer Polystyrene Styrene–acrylonitrile copolymers Styrene–acrylonitrile–butadiene copolymers Sulfones: polysulfone Vinyls: poly(vinyl chloride)	E N G E	E N N G	E E N G F E	E F G	E N N G E	G N N N N	N F F	E E F G F	G N N F F G	F N N N	N N N N	G N N N	F N G G
Natural rubber Nitrile rubber Polychloroprene Polyisobutylene Polysulfide rubbers: Thiokol Styrene–butadiene rubber			E E E E E			N N N F E	N G F E N	E E E E E	N E F N E	N N N N F	N N N N	N N N N N	

TABLE 10.5 Common Abbreviations Used in Polymer Chemistry

Acronym	Expansion
ABA	Acrylonitrile-butadiene-acrylate
ABS	Acrylonitrile-butadiene-styrene copolymer
ABS-PC	Acrylonitrile-butadiene-styrene-polycarbonate alloy
ABS-PVC	Acrylonitrile-butadiene-styrene-poly(vinyl chloride) alloy
ACM	Acrylic acid ester rubber
ACS	Acrylonitrile-chlorinated pe-styrene
AES	Acrylonitrile-ethylene-propylene-styrene
AMMA	Acrylonitrile-methyl methacrylate
AN	Acrylonitrile
APET	Amorphous polyethylene terephthalate
APP	Atactic polypropylene
ASA	Acrylic–styrene–acrylonitrile
BR	Butadiene rubber
BS	Butadiene styrene rubber
CA	Cellulose acetate
CAB	Cellulose acetate-butyrate
CAP	Cellulose acetate–propionate
CN	Cellulose nitrate
CP	Cellulose propionate
CPE	Chlorinated polyethylene
CPET	Crystalline polyethylene terephthalate
CPP	Cast polypropylene
CPVC	Chlorinated polyvinyl chloride
CR	Chloroprene rubber
CTA	Cellulose triacetate
DAM	Diallyl maleate
DAP	Diallyl phthalate
DMT	Terephthalic acid, dimethyl ester
ECTFE	Ethylene–chlorotrifluoroethylene copolymer
EEA	Ethylene–ethyl acrylate
EMA	Ethylene–methyl acrylate
EMAA	Ethylene methacrylic acid
EMAC	Ethylene–methyl acrylate copolymer
EMPP	Elastomer modified polypropylene
EnBA	Ethylene normal butyl acrylate
EP	Epoxy resin, also ethylene–propylene
EPM	Ethylene–propylene rubber
ESI	Ethylene–styrene copolymers
EVA(C)	Polyethylene–vinyl acetate
EVOH	Polyethylene–vinyl alcohol copolymers
FEP	Fluorinated ethylene–propylene copolymers
HDI	Hexamethylene diisocyanate
HDPE	High-density polyethylene
HIPS	High-impact polystyrene
HMDI	Diisocyanato dicyclohexylmethane
IPI	Isophorone diisocyanate
LDPE	Low-density polyethylene
LLDPE	Linear low-density polyethylene Linear low-density polyethylene
MBS	Methacrylate—butadiene—styrene
MIDS	iviculaci ylate—butatiene—stylene

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TABLE 10.5 Common Abbreviations Used in Polymer Chemistry (continued)

Acronym	Expansion
MC	Methyl cellulose
MDI	Methylene diphenylene diisocyanate
MEKP	Methyl ethyl ketone peroxide
MF	Melamine formaldehyde
MMA	Methyl methacrylate
MPEG	Polyethylene glycol monomethyl ether
MPF	Melamine-phenol-formaldehyde
NBR	Nitrile butyl rubber
NDI	Naphthalene diisocyanate
NR	Natural rubber
OPET	Oriented polyethylene terephthalate
OPP	Oriented polypropylene
OSA	Olefin-modified styrene-acrylonitrile
PA	Polyamide
PAEK	Poly(aryl ether–ketone)
PAI	Poly(amide-imide)
PAN	Polyacrylonitrile
PB	Polybutylene
PBAN	Poly(butadiene–acrylonitrile)
PBI	Polybenzimidazole
PBN	Polybutylene naphthalate
PBS	Poly(butadiene–styrene)
PBT	Poly(butylene terephthalate)
PC	Polycarbonate
PCD	Polycarbodiimide
PCT	Poly(cyclohexylene–dimethylene terephthalate)
PCTFE	Polychlorotrifluoroethylene
PE	Polyethylene
PEC	Chlorinated polyethylene
PEG	Poly(ethylene glycol)
PEI	Poly(ether–imide)
PEK	Poly(ether–ketone)
PEN	Polyethylene naphthalate
PES	Polyether sulfone
PET	Polyethylene terephthalate
PF	Phenol-formaldehyde copolymer
PFA	Perfluoroalkoxy resin
PI	Polyimide
PIBI	Poly(isobutylene), Butyl rubber
PMDI	Polymeric methylene diphenylene diisocyanate
PMMA	Poly(methyl methacrylate)
PMP	Poly(methylpentene)
PO	Polyolefins
PP	Polypropylene
PPA	Polyphthalamide
PPC	Chlorinated polypropylene
PPO	Poly(phenylene oxide)
110	
PPS	Poly(phenylene sulfide)

TABLE 10.5 Common Abbreviations Used in Polymer Chemistry (*continued*)

Acronym	Expansion
PS	Polystyrene
PSF	Polysulfone (also PSU)
PSU	Polysulfone (also PSF)
PTFE	Polytetrafluoroethylene
PU	Polyurethane
PUR	Polyurethane
PVA	Poly(vinyl acetate)
PVAL	Poly(vinyl alcohol)
PVB	poly(vinyl butyrate)
PVC	Poly(vinyl chloride)
PVCA	Poly(vinyl chloride–acetate)
PVDA	Poly(vinylidene acetate)
PVDC	Poly(vinylidene chloride)
PVDF	Poly(vinylidene fluoride)
PVF	Poly(vinyl fluoride)
PVOH	Poly(vinyl alcohol)
SAN	Styrene–acrylonitrile copolymer
SB	Styrene-butadiene copolymer
SBC	Styrene block copolymer
SBR	Styrene butadiene rubber
SMA	Styrene-maleic anhydride (also SMC)
SMC	Styrene–maleic anhydride (also SMA)
TA	Terephthalic acid (also TPA)
TDI	Toluene diisocyanate
TEFE	Ethylene-tetrafluoroethylene copolymer
TPA	Terephthalic acid (also TA)
UF	Urea formaldehyde
ULDPE	Ultralow-density polyethylene
UP	Unsaturated polyester resin
UR	Urethane
VLDPE	Very low-density polyethylene
ZNC	Ziegler-Natta catalyst

TABLE 10.6 Gas Permeability Constants $(10^{10}P)$ at 25 °C for Polymers and Rubbers

The gas permeability constant P is defined as

$$P = \frac{\text{amount of permeant}}{(\text{area}) \times (\text{time}) \times (\text{driving forced across the film})}$$

The gas permeability constant is the amount of gas expressed in cubic centimeters passed in 1 s through a 1-cm² area of film when the pressure across a film thickness of 1 cm is 1 cmHg and the temperature is $25\,^{\circ}$ C. All tabulated values are multiplied by 10^{10} and are in units of seconds⁻¹ (centimeters of Hg)⁻¹. Other temperatures are indicated by exponents and are expressed in degrees Celsius.

					Gas		
Polymer or rubber	Не	N_2	H_2	O_2	CO ₂	$\rm H_2O$	Other
Cellulose (cellophane)	0.005^{20}	0.0032	0.0065	0.0021	0.0047	1900	0.006 ⁴⁵ (H ₂ S); 0.0017 (SO ₂)
Cellulose acetate	13.620	0.28^{30}	3.5^{20}	0.7830	22.730	5 500	3.5 ³⁰ (H ₂ S); 17 ⁰ (ethylene oxide); 6.8 ⁶⁰ (bromomethane)
Cellulose nitrate	6.9	0.12	2.0^{20}	1.95	2.12	6290	57.1 (NH ₃); 1.76 (SO ₂)
Ethyl cellulose	40030	8.430	8720	26.530	41.030	12000^{20}	705 (NH ₃); 204 (SO ₂); 420 ⁰ (ethylene oxide)
Gutta percha		2.17	14.4	6.16	35.4	510	
Natural rubber		9.43	52.0	23.3	15.3	2290	15.7 (CO); 30.1 (CH ₄); 1.68 (C ₃ H ₈); 98.9 (C ₂ H ₂); 550 (CH ₃ C≡CH); 3.59 (SF ₆)
Nylon 6	0.53 ²⁰	0.0095^{30}		0.03830	0.10^{30}	177	0.33 ³⁰ (H ₂ S); 1.2 ²⁰ (NH ₃); 0.84 ⁶⁰ (CH ₃ Br)
Nylon 11	1.95 ³⁰		1.7830		1.0040		0.344 ³⁰ (Ne); 0.189 ⁴⁰ (Ar); 13.6 ⁵⁰ (propyne)
Poly(acrylonitrile)				0.0002	0.0008	300	4 10

Acrylonitrile–styrene copolymer (66:34)		6.40	41.0	0.048	0.21	2000	
Poly(1,3-butadiene)	22.6	6.42 19.2	41.9	19.0	138.0	5070	10.2 (N-): 41.0 (A-)
Poly(<i>cis</i> -1,4-butadiene) Butadiene–acrylonitrile copolymer	32.6	19.2					19.2 (Ne); 41.0 (Ar)
(80:20)	12.2	1.06	15.9	3.85	30.8		24.8 (C ₂ H ₂); 7.7 (propyne)
Butadiene–styrene copolymer (80:20)	13.4	1.71	13.7	3.03	50.0		5.01 (Ne); 4.49 (Ar)
Butadiene–styrene copolymer (92:8)	22.9	5.11					9.70 (Ne); 12.7 (Ar)
Polychloroprene		1.2	13.6	4.0	25.8		3.79 (Ar); 3.27 (CH ₄)
Polyethylene, low-density	4.9	0.969	12.030	2.88	12.6	90	2.88 (CH ₄); 6.81 (C ₂ H ₆);
							9.43 (C ₃ H ₈); 1.48 (CO);
							49 ⁰ (ethylene oxide);
							14.4 (propene); 42.2 (propyne);
			20				$0.170 (SF_6); 472^{60} (CH_3Br)$
Polyethylene, high-density	1.14	0.143	3.0^{20}	0.403	0.36	12.0	0.388 (CH ₄); 0.590 (C ₂ H ₆);
							0.537 (C ₃ H ₈); 0.0083 (SF ₆);
Daly (athylana tananhthalata)							1.69 (Ar); 4.01 (propene)
Poly(ethylene terephthalate) Crystalline	1.32	0.0065	3.70^{20}	0.035	0.17	130	0.003 2 (CH ₄); 0.08 ⁶⁰ (CH ₃ Br)
Amorphous	3.28	0.0003	3.70	0.059	0.17	130	0.0032 (CH ₄), 0.08 (CH ₃ BI) 0.009 (CH ₄)
Poly(ethyl methacrylate)	6.82	0.220		1.15	5.00	3 200	2.98 (Ne); 0.565 (Ar); 0.370 (Kr);
1 org (enry 1 meanur) mice)	0.02	0.220		1.10	2.00	3200	3.83 (H ₂ S); 0.00000165 (SF ₆)
Isobutene-isoprene copolymer							247, 111111111111111111111111111111111111
(98:2)	8.38	0.324	7.20	1.30	5.16	110^{38}	$13.6^{50} (C_3H_8)$
Isoprene-acrylonitrile copolymer							
(76:24)	7.77	0.181	7.41	0.852	4.32		
	'		•	•	•	'	•

TABLE 10.6 Gas Permeability Constants $(10^{10}P)$ at 25 °C for Polymers and Rubbers (*continued*)

		Gas										
Polymer or rubber	Не	N ₂	H_2	O_2	CO ₂	H ₂ O	Other					
Isoprene–methacrylonitrile copolymer (76:24) Methacrylonitrile–styrene– butadiene copolymer (88:7:5) Poly(methylpentene) Polypropylene Silicone rubber, 10% filler	$ \begin{array}{c} 101 \\ 38^{20} \\ 233^{0} \end{array} $	0.596 7.83 0.44 ³⁰ 227 ⁰	13.6 136 41 ²⁰ 464 ⁰	2.34 0.0048 32.0 2.3 ³⁰ 489 ⁰	14.1 0.014 92.6 9.2 ³⁰ 3240	600 51 43 000 ³⁵	0.33 ²⁰ (H ₂ S); 9.2 ²⁰ (NH ₃) 191 ⁰ (Ne); 550 ⁰ (Ar);					
Sincone rubber, 10% liner	255	221	404	409	3 240	43000	191 (Ne), 330 (A1), 1020 ⁰ (Kr); 2550 ⁰ (Xe); 19000 ⁰ (butane)					
Polystyrene Poly(tetrafluoroethylene)	18.7	0.788	23.3 9.8	2.63 4.2	10.5 11.7	1200	15.7 (NO ₂); 37.5 (N ₂ O ₄)					
Poly(trifluoroethylene) Poly(vinyl acetate)	6.8^{20} 12.6^{30}	0.003	0.94^{20} 89^{30}	0.025^{40} 0.50^{30}	0.048^{40}	0.29	1.2 ⁰ (ethylene oxide); 4.6 ⁶⁰ (CH ₃ Br) 2.64 ³⁰ (Ne); 0.19 ³⁰ (Ar);					
Poly(vinyl alcohol)	0.001^{30}	< 0.00114	0.009	0.0089	0.001^{23}		0.078 ³⁰ (Kr); 0.050 ³⁰ (CH ₄) 0.007 (H ₂ S); 0.002 ⁰ (ethylene oxide)					
Poly(vinyl chloride)	2.05	0.0118	1.70	0.0453	0.157	275	3.92 (Ne); 0.0115 (Ar); 0.0286 (CH ₄)					
Poly(vinylidene chloride)	0.3134	0.00094^{30}		0.0053^{30}	0.03^{30}	0.5	0.03 ³⁰ (H ₂ S); 0.008 ⁶⁰ (CH ₃ Br)					

TABLE 10.7 Vapor Permeability Constants $(10^{10}P)$ at 35 °C for Polymers All tabulated values are multiplied by 10^{10} and are in units of seconds⁻¹ (centimeters of Hg)⁻¹.

		Vapor							
Polymer	Benzene	Hexane	Carbon tetrachloride	Ethanol	Ethyl acetate				
Cellulose	1.4	0.912	0.836	85.8	13.4				
Cellulose acetate	512	2.80	3.74	2980	3 5 9 5				
Poly(acrylonitrile)	2.61	1.59	1.47	0	1.34				
Polyethylene, low-density	5 3 0 0	2910	3810	55.9	513				
Polystyrene	10600		6820	0	soluble				
Poly(vinyl alcohol)	3.58	2.34	1.61	32.7	2.53				

FATS, OILS, AND WAXES

TABLE 10.8 Constants of Fats and Oils

Fat or oil	Solidification point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value					
Animal origin											
Butterfat Chicken fat Cod-liver oil Deer fat	20–23 21–27 –3	0.91_{15}^{40} °C 0.924 0.92– $0.930.96$ – 0.97	1.455 0.925 ²⁵ °C	0.5–35 1.2 5.6 0.8–5.3	210–230 193–205 171–189 195–200	26–38 66–72 137–166 26–36					

TABLE 10.8 Constants of Fats and Oils (*continued*)

Fat or oil	Solidification point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value
		Animal o	origin (continued)			
Dolphin	-3 to +5	0.91-0.93		2–12	203 (body); 290 (jaw)	127 (body); 33 (jaw)
Goat butter		$0.91 - 0.94^{38}_{38}^{\circ}C$			233–236	25–37
Goose fat	22–24	0.92-0.93		0.6	191–193	58–67
Herring oil		0.92-0.94	0.900 ⁶⁰ °C	1.8-44	170–194	102-149
Horse fat	20–45	0.92-0.93		0-2.4	195-200	75–86
Human fat	15	0.903	1.460		193-200	57–73
Lard oil	-2 to +4	0.913-0.915	1.462	0.1-2.5	193-198	63–79
Lard oil, fatty tissue	27–30	0.93-0.94	1.462	0.5-0.8	195-203	47–67
Menhaden oil	-5	0.92-0.93	1.465 ⁶⁰ °C	3–12	189-193	148-185
Neat's-foot oil	-2 to +10	0.91-0.92	1.464 ²⁵ ℃	0.1-0.6	193-199	58–75
Porpoise, body oil	-16	0.926		1.2	203	127
Rabbit fat	17–23	0.93-0.94		1.4-7.2	199-203	70–100
Sardine oil	20–22	0.92-0.93	1.466 ⁶⁰ °C	4-25	188-196	130-152
Seal	3	0.915-0.926		1.9-40	188-196	130-152
Shark		0.916-0.919			157-164	115-139
Sperm oil	15.5	0.878-0.884		13	120-137	80–84
Tallow, beef	31–38	0.895		0.25	196-200	35–42
Tallow, mutton	32–41	0.937-0.953	1.457 ⁴⁰ °C	2-14	195-196	48-61
Whale oil	-2 to 0	0.917-0.924	1.460 ⁶⁰ °C	1.9	160–202	90–146
		Plai	nt origin			
Acorn	-10	0.916			199	100
Almond	-20 to -15	0.914-0.921		0.5-3.5	183–208	93-103

Babassu oil	22-26	0.893 ⁶⁰ °C	1.443 ⁶⁰ °C		247	16
Beechnut oil	-17	0.922			191-196	97–111
Castor oil	-18 to -17	0.960-0.967	1.477	0.1-0.8	175–183	84
Chaulmoogra oil, USP	<-25	0.950 ^{25°C}			196-213	98-110
Chinese vegetable tallow	24-34	0.918-0.922		2.4	179-206	23-41
Cocoa butter	21.5-23	0.964-0.974	1.457 ⁴⁰ °C	1.1-1.9	193-195	33–42
Coconut oil	14-22	0.926	1.449 ⁴⁰ °C	2.5-10	153-262	6–10
Corn (maize) oil	-20 to -10	0.921-0.928	1.473 ⁴⁰ ℃	1.4-2.0	187-193	111-128
Cottonseed oil	-13 to +12	0.918 ^{25°C}	1.474 ⁴⁰ °C	0.6-0.9	194-196	103-111
Hazelnut oil	-18 to -17	0.917			191-197	87
Hemp-seed oil	-28 to -15	0.928-0.934		0.45	190-195	145-162
Linseed oil	-27 to -19	0.930-0.938	1.478 ^{25 ℃}	1-3.5	188-195	175–202
Mustard oil, black	16	0.918-0.921	1.475 ⁴⁰ °C	5.7-7.3	173–175	99-110
Neem oil	-3	0.917	1.462 ⁴⁰ °C		195	71
Niger-seed oil		0.925	1.471 ⁴⁰ °C		190	129
Oiticica oil		0.974 ²⁵ °C				140-180
Olive oil	-6	0.914-0.918	1.468 ⁴⁰ °C	0.3 - 1.0	185-196	79–88
Palm oil	35-42	0.915	1.458 ⁴⁰ °C	10	200-205	49–59
Palm kernel oil	24	0.918-0.925	1.457 ⁴⁰ ℃	0.3-0.6	220-231	26–32
Peanut oil	3	0.917-0.926	1.469 ⁴⁰ °C	0.8	186-194	88–98
Perilla oil		0.930-0.937	1.481 ^{25 ℃}		188-194	185-206
Pistachio-nut oil	-10 to -5	0.913-0.919			191	83–87
Poppy-seed oil	-18 to -16	0.924-0.926	1.469⁴0°C	2.5	193-195	128-141
Pumpkin-seed oil	-15	0.923-0.925			188-193	121-130
Rapeseed oil	-10	0.913-0.917	1.471 ⁴⁰ °C	0.36-1.0	168-179	94–105
Safflower oil	-18 to -13	0.925-0.928	1.462 ⁶⁰ °C	0.6	188-203	122-141
Sesame oil	-6 to -4	0.919 ^{25°C}	1.465 ⁴⁰ °C	9.8	188-193	103-117
Soybean oil	-16 to -10	0.924-0.927	1.473 ⁴⁰ ℃	0.3 - 1.8	189-194	122-134
Sunflower-seed oil	-17	0.924-0.926	1.469 ⁴⁰ °C	11.2	188-193	129-136
Tung oil	-2.5	0.94-0.95	1.517 ²⁵ ℃	2	190–197	163-171
White-mustard-seed oil	-16 to -8	0.912-0.916		5.4	171–174	94–98
Wheat-germ oil						125

TABLE 10.9 Constants of Waxes

Wax	Melting point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value
Bamboo leaf	79–80	0.961 ^{25°C}		14–15	43–44	7.8
Bayberry (myrtle)	47–49	0.99	1.436 ^{80 °C}	3–4	205–212	4–9.5
Beeswax, ordinary	62–66	0.95-0.97	1.44-1.48 ⁴⁰ °C	17–21	88-100	8-11
Beeswax, East Indian	61–67	0.95-0.97	1.44 ⁴⁰ °C	5-10.5	87–117	4–10.5
Beeswax, white, USP	61–69	0.95-0.98	1.45–1.47 ⁶⁵ °C	17–24	90–96	7–11
Candelilla	73–77	0.98-0.99	1.45-1.46 ^{85 °C}	19–24	55-64	14–20
Cape berry	40-45	1.01	1.45 ⁴⁵ °C	2.5-4.0	211–215	0.5-2.5
Caranda	80–85	0.99-1.00		5.0-9.5	64–79	8–9
Carnauba, No. 1 yellow	86–88	0.99-1.00		1.5-2.5	75–86	
Carnauba, No. 3, crude	86–90	0.99-1.01		3.0-8.5	75–89	
Carnauba, No. 3, refined	86–89	0.96-0.97	1.47 ⁴⁰ °C	3.0-5.0	76–85	7–13.5
Castor oil, hydrogenated	83-88	0.98-0.99 ²⁰ °C		1.0-5.0	177-181	2.5-8.5
Chinese insect	80–85	0.95-0.97	1.46 ⁴⁰ °C	2–9	78–93	1.0-2.5
Cotton	68-71	0.96		32	71	25
Cranberry	207-218	0.97-0.98		42-59	131–134	44–53
Esparto	75–79	0.985-0.995		22–27	58–73	7–15

Flax Japan Jojoba Microcrystalline, amber Microcrystalline, white Montan, crude Montan, refined Ouricury Ozokerite Palm Paraffin, American Shellac Sisal hemp	61-70 49-56 11-12 64-91 71-89 76-86 77-84 86-89 56-82 74-86 49-63 79-82 74-81	0.91–0.99 0.97–1.00 0.86–0.90 ^{25°C} 0.91–0.94 0.93–0.94 1.01–1.02 ^{25°C} 1.02–1.04 0.99–1.01 0.90–1.00 0.99–1.05 0.896–0.925 0.97–0.98 1.007–1.010	1.465 ^{25°C} 1.42–1.45 ^{80°C} 1.441 ^{80°C} 1.44–1.48 ^{80°C}	17–48 4–15 0.2–0.6 0 0 22–31 23–45 12–19 0 5–11 0 12–24 16–19	37-102 210-235 92-95 0 0 59-92 72-115 88-96 0 64-104 0 64-83 56-58	22–29 4–15 82–88 0 0 14–18 10–14 6.9–7.8 4–8 9–17 0 6–9 28–29
Shellac	79–82	0.97-0.98	1.44–1.48 ^{80°C}	12–24	64–83	6–9
Sisal hemp Spermaceti Sugarcane, refined Wool	74–81 41–49 76–82 38–40	1.007–1.010 0.905–0.960 0.96–0.98 0.97	1.51 ²⁵ °C 1.48 ⁴⁰ °C	0.5–3.0 8–23 6–22	56–58 121–135 55–70 82–130	28–29 2.5–8.5 13–29 15–47

SECTION 11

ABBREVIATIONS, CONSTANTS, AND CONVERSION FACTORS

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11.2 SECTION 11

PHYSICAL CONSTANTS

 TABLE 11.1
 Fundamental Physical Constants

A. Defined values

Name of unit	Symbol	Definition
		SI base units
Meter (metre) (preferred spelling in U.S. is meter)	m	1 650 763.73 wavelengths in vacuum of the orange-red line of the spectrum of krypton-86
Kilogram Second	kg s	Mass of a cylinder of platinum–iridium alloy kept at Paris Duration of 9 192 631 770 cycles of the radiation associated with a specified transition of the cesium atom
Ampere	A	Magnitude of the current that, when flowing through each of two long parallel wires separated by one meter in free space, results in a force between the two wires 2×10^{-7} newton for each meter of length
Kelvin (degree Kelvin)	K	Defined in the thermodynamic scale by assigning 273.16 K to the triple point of water (freezing point, 273.15 K = 0° C)
Candela	cd	Luminous intensity of 1/600000 of a square meter of a radiating cavity at the temperature of freezing platinum (2042 K)
Mole	mol	Amount of substance which contains as many specified entities (molecules, atoms, ions, electrons, photons, etc.) as there are atoms of carbon-12 in exactly 0.012 kg of that nuclide
		Supplementary SI units
Radian	rad	The plane angle between two radii of a circle which cut off on the circumference an arc equal in length to the radius
Steradian	sr	The solid angle which, having its vertex in the center of a sphere, cuts off an area of the surface of the sphere equal to that of a square with sides of length equal to the radius of the sphere

B. Derived SI units

Quantity and symbol	Name of SI unit	Symbol and definition
Capacitance (electric), <i>C</i> Charge (electric), quantity of	farad	$F = C \cdot V^{-1}$
electricity, Q Conductance (electric), $G(=1/R)$ Energy, work, quantity of heat, H	coulomb siemens joule	$C = A \cdot s$ $S = \Omega^{-1}$ $J = kg \cdot m^2 \cdot s^{-2}$

TARIF 11 1	Fundamental Physical Constants	(continued)

Quantity and symbol	Name of SI unit	Symbol and definition		
Force	newton	$N = kg \cdot m \cdot s^{-2}$		
Frequency	hertz	$Hz = s^{-1}$		
Illuminance, illumination	lux	$1x = 1m \cdot m^{-2}$		
Inductance, L	henry	$H = \Omega \cdot s$		
Luminous flux	lumen	$lm = cd \cdot sr$		
Magnetic flux	weber	$Wb = V \cdot s$		
Magnetic flux density	tesla	$T = Wb \cdot m^{-2}$		
Potential difference, E	volt	$V = kg \cdot m^2 \cdot s^{-3} \cdot A^{-1} = J \cdot A^{-1} \cdot s^{-1}$		
Power, radiant flux	watt	$W = kg \cdot m^2 \cdot s^{-3} = J \cdot s^{-1}$		
Pressure, stress	pascal	$Pa = N \cdot m^{-2} = kg \cdot m^{-1} \cdot s^{-2}$		
Resistance (electric), R	ohm	$\Omega = \mathbf{V} \cdot \mathbf{A}^{-1} = \mathbf{kg} \cdot \mathbf{m}^2 \cdot \mathbf{s}^{-3} \cdot \mathbf{A}^{-2}$		

C. Recommended Consistent Values of Constants

Constant

Gravitational constant

The digits in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digits.

Symbol and value

= 82.0568(26) cm³ · atm · mol⁻¹ · K⁻¹ = 1.987 19(6) cal · mol⁻¹ · K⁻¹ $G = 6.672(4) \times 10^{-11} \text{ N} \cdot \text{m}^2 \cdot \text{kg}^{-2}$

Anomalous electron moment $(\mu_e/\mu_0) - 1 = 1.159615(15) \times 10^{-3}$ correction $u = (10^{-3} \text{kg} \cdot \text{mol}^{-1})/N_4 = 1.660566(9) \times 10^{-27} \text{kg}$ Atomic mass unit $N_A = 6.022045(31) \times 10^{23} \,\mathrm{mol}^{-1}$ Avogadro constant $\mu_{R} = e\hbar/2m_{e}c = 9.274078(36) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$ Bohr magneton Bohr radius $a_0 = \alpha/4\pi R_m = 0.52917706(44) \times 10^{-10} \text{ m}$ $k = R/N_A = 1.380662(44) \times 10^{-23} \,\text{J} \cdot \text{K}^{-1}$ Boltzmann constant $e/m_e = 1.758805(5) \times 10^{11} \,\mathrm{C} \cdot \mathrm{kg}^{-1}$ Charge-to-mass ratio for electron $\lambda_c = \alpha^2 / 2R_\alpha = 2.426309(4) \times 10^{-12} \,\mathrm{m}$ Compton wavelength of electron $\chi_c = \lambda_c/2\pi = \alpha a_0 = 3.861591(6) \times 10^{-13} \,\mathrm{m}$ $\lambda_{c,n} = h/m_n c = 1.319591(2) \times 10^{-15} \,\mathrm{m}$ Compton wavelength of neutron Compton wavelength of proton $\lambda_{c,p} = h/m_p c = 1.321410(2) \times 10^{-15} \text{ m}$ Diamagnetic shielding factor, $1 + \sigma(H_2O) = 1.00002564(7)$ spherical H2O molecule $g_a/2 = \mu_a/\mu_B = 1.001159657(4)$ Electron g-factor Electron magnetic moment $\mu_e = 9.284832(36) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$ Electron radius (classical) $\alpha \chi_c = \mu_0 e^2 / 4\pi m_e = r_e = 2.817938(7) \times 10^{-15} \,\mathrm{m}$ $m_e = 0.910953(5) \times 10^{-30} \text{kg}$ Electron rest mass $= 5.485803(2) \times 10^{-4} \mathrm{u}$ $e = 1.602189(5) \times 10^{-19}$ C Elementary charge $N_4 e = F = 9.648456(27) \times 10^4 \text{ C} \cdot \text{mol}^{-1}$ Faraday constant $\mu_0 ce^2/2h = \alpha = 0.007297351(6)$ Fine structure constant $1/\alpha = 1.370360(1)$ First radiation constant $2\pi hc^2 = c_1 = 3.74183(2) \times 10^{-16} \,\mathrm{W} \cdot \mathrm{m}^2$ $R = P_0 V_m / T_0 = 8.31441(26) \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ Gas constant (molar)

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TABLE 11.1 Fundamental Physical Constants (*continued*)

Constant	Symbol and value
Gyromagnetic ratio of proton	$\gamma_p = 2.675199(8) \times 10^8\mathrm{s}^{-1}\cdot\mathrm{T}^{-1}$
(uncorrected for	
diamagnetism of H ₂ O)	$\gamma_p' = 675130(8) \times 10^8 \mathrm{s}^{-1} \cdot \mathrm{T}^{-1}$
Josephson frequency-voltage ratio	$2e/h = 4.835939(13) \times 10^{14} \text{Hz} \cdot \text{V}^{-1}$
Magnetic flux quantum	$\Phi_0 = h/2e = 2.067851(5) \times 10^{-15} \text{Wb}$
Molar standard volume, ideal gas	$V_m = RT_0/P_0 = 0.0224138(7) \mathrm{m}^3 \cdot \mathrm{mol}^{-1}$
Muon g-factor	$e\hbar/2m_{\mu}c = g_{\mu}/2 = 1.00116616(31)$
Muon magnetic moment	$\mu_{\mu} = 4.490474(18) \times 10^{-26} \mathrm{J} \cdot \mathrm{T}^{-1}$
Muon rest mass	$m_{\mu} = 1.883566(11) \times 10^{-28}\mathrm{kg}$
Neutron rest mass	$m_n = 1.674954(9) \times 10^{-27} \text{kg}$
Normal volume, perfect gas	$V_0 = 2.24136(30) \times 10^4 \text{cm}^3 \cdot \text{mol}^{-1}$
Nuclear magneton	$\mu_N = e\hbar/2m_p c = 5.050824(20) \times 10^{-27}\mathrm{J}\cdot\mathrm{T}^{-1}$
Permeability of vacuum	$\mu_0 = 4\pi \times 10^{-7} \mathrm{H} \cdot \mathrm{m}^{-1}$
Permittivity of vacuum	$\varepsilon_0 = (\mu_0 c^2)^{-1} = 8.85418782(7) \times 10^{-12} \text{F} \cdot \text{m}^{-1}$
Planck constant	$h = 6.626176(36) \times 10^{-34} \mathrm{J \cdot s}$
	$\hbar = h/2\pi = 1.054589(6) \times 10^{-34} \text{J} \cdot \text{s}$
Proton magnetic moment:	$\mu_p = 1.410617(5) \times 10^{-26} \mathrm{J} \cdot \mathrm{T}^{-1}$
In Bohr magnetons	$\mu_p/\mu_B = 1.521032209(16) \times 10^{-3}$
In nuclear magnetons	$\mu_p/\mu_N = 2.7928456(11)$
Proton rest mass	$m_p = 1.672649(9) \times 10^{-27} \text{kg}$
Quantum-charge ratio	$h/e = 4.135701(11) \times 10^{-15} \text{J} \cdot \text{Hz}^{-1} \cdot \text{C}^{-1}$
Quantum of circulation	$h/m_e = 7.27389(1) \times 10^{-4}\mathrm{J}\cdot\mathrm{s}\cdot\mathrm{kg}^{-1}$
Ratio, electron to proton	
magnetic moments	$\mu_e/\mu_p = 6.58210688(7) \times 10^2$
Ratio, kxu (Siegbahn) to	
angstrom	= 1.0000205(56)
Ratio, muon moment to proton	
moment	$\mu_{\mu}/\mu_{p} = 3.183340(7)$
Rydberg constant	$R_{\infty} = 1.09737318(8) \times 10^7 \mathrm{m}^{-1}$
Second radiation constant	$c_2 = hc/k = 1.438786(45) \times 10^{-2} \mathrm{m \cdot K}$
Speed of light in vacuum	$c = 2.99792458(12) \times 10^8 \mathrm{m \cdot s^{-1}}$
Stefan-Boltzmann constant	$\sigma = (\pi^2/60)k^4/\hbar^3c^2 = 5.6703(7) \times 10^{-8} \mathrm{W} \cdot \mathrm{m}^{-2} \cdot \mathrm{K}^{-4}$
Thomson cross section	$\sigma_e = 8\pi r_e^2/3 = 6.652448(33) \times 10^{-28} \mathrm{m}^2$
Voltage-wavelength product	$V\lambda = 1.239852(3) \times 10^{-6} \text{eV} \cdot \text{m}$
Wien displacement constant	$b = 0.28978(4) \mathrm{cm} \cdot \mathrm{K}$
Zeeman splitting constant	$\mu_B/hc = 4.66858(4) \times 10^{-5} \mathrm{cm}^{-1} \cdot \mathrm{G}^{-1}$
Energy equivalents:	
1 atomic mass unit	u = 931.5016(26) MeV
1 proton mass	$m_{\nu} = 938.2796(27) \mathrm{MeV}$
1 neutron mass	$m_n = 939.5731(27) \mathrm{MeV}$
1 muon mass	$m_{\mu} = 105.65948(35) \mathrm{MeV}$
1 electron mass	$m_e = 0.5110034(14) \mathrm{MeV}$
1 electronvolt	$1 \mathrm{eV}/k = 1.160450(36) \times 10^4 \mathrm{K}$
	$1 \text{ eV/}hc = 8.065479(21) \times 10^3 \text{ cm}^{-1}$
	$1 \mathrm{eV}/h = 2.417970(6) \times 10^{14} \mathrm{Hz}$

GREEK ALPHABET

TABLE 11.2 Greek Alphabet

Capital	Lowercase	Letter	Capital	Lowercase letter	Letter
letter	letter	name	letter		name
Α	α	Alpha	N	ν	Nu
Β	β	Beta	Ξ	ξ	Xi
Γ	γ	Gamma	О	ο	Omicron
Δ	δ	Delta	П	π	Pi
E	arepsilon $arepsilon$ $arepsilon$ $artheta$	Epsilon	P	ρ	Rho
Z		Zeta	Σ	σ	Sigma
H		Eta	Τ	τ	Tau
Θ		Theta	Υ	υ	Upsilon
I	ι	Iota	Φ	$\phi \ \chi \ \psi \ \omega$	Phi
Κ	κ	Kappa	X		Chi
Λ	λ	Lambda	Ψ		Psi
Μ	μ	Mu	Ω		Omega

PREFIXES

TABLE 11.3 Prefixes for Naming Multiples and Submultiples of Units

For example: 10^{-9} gram is one nanogram, or 1 ng.

Factor	Prefix	Symbol	Factor	Prefix	Symbol
1012	tera	Т	10^{-2}	centi	c
10^{9}	giga	G	10^{-3}	milli	m
10^{6}	mega	M	10^{-6}	micro	μ
10^{3}	kilo	k	10^{-9}	nano	n
10^{2}	hecto	h	10^{-12}	pico	p
10	deka	da	10^{-15}	femto	f
10^{-1}	deci	d	10^{-18}	atto	a

TABLE 11.4 Numerical Prefixes

Number	Prefix	Number	Prefix	Number	Prefix
$ \frac{1}{2} $ 1 1 $ \frac{1}{2} $ 2 3 4	hemi mono sesqui di or bi tri tetra	6 7 8 9 10	hexa hepta octa nona deca undeca	13 14 15 16 17 18	trideca tetradeca pentadeca hexadeca heptadeca octadeca
5	penta	12	dodeca	19	nonadeca

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TABLE 11.4 Numerical Prefixes (continued)

Number	Prefix	Number	Prefix	Number	Prefix
20	icosa	34	tetratriaconta	48	octatetraconta
21	henicosa	35	pentatriaconta	49	nonatetraconta
22	docosa	36	hexatriaconta	50	pentaconta
23	tricosa	37	heptatriaconta	51	henpentaconta
24	tetracosa	38	octatriaconta	52	dopentaconta
25	pentacosa	39	nonatriaconta	53	tripentaconta
26	hexacosa	40	tetraconta	54	tetrapentaconta
27	heptacosa	41	hentetraconta	55	pentapentaconta
28	octacosa	42	dotetraconta	56	hexapentaconta
29	nonacosa	43	tritetraconta	57	heptapentaconta
30	triaconta	44	tetratetraconta	58	octapentaconta
31	hentriaconta	45	pentatetraconta	59	monapentaconta
32	dotriaconta	46	hexatetraconta	60	hexaconta
33	tritriaconta	47	heptatetraconta		

TRANSFORMATIONS

TABLE 11.5 Conversion Formulas for Solutions Having concentrations expressed in Various Ways

Abbreviations Used in the Table

 $\begin{array}{ll} \text{wt \%, weight percent of solute} & \textit{m, molality} \\ \text{MW}_1, \text{molecular weight of solute} & \textit{M, molarity} \\ \text{MW}_2, \text{molecular weight of solvent} & \textit{n, mole fraction} \\ \end{array}$

d, density of solution (g·mL⁻¹) G, grams of solute per liter of solution

To obtain	From	Compute		
molarity	weight per cent of solute	$M = \frac{10 d(\text{wt \%})}{\text{MW}_1}$		
molarity	molality	$M = \frac{1000 \ dm}{1000 + (MW_1)m}$		
molarity	grams of solute per liter of solution	$M = \frac{G}{MW_1}$		
molarity	mole fraction	$M = \frac{1000 dn}{n(\text{NW}_1) + \text{MW}_2(1-n)}$		
mole fraction	weight per cent of solute	$n = \frac{(\text{wt \%})/\text{MW}_1}{(\text{wt \%})/\text{MW}_1 + (100 - \text{wt \%})\text{MW}_2}$		
mole fraction	molality	$n = \frac{(MW_2)m}{(MW_2)m + 1000}$		
mole fraction	molarity	$n = \frac{M(MW_2)}{M(MW_2 - MW_1) + 1000 d}$		

TABLE 11.5 Conversion Formulas for Solutions Having concentrations expressed in Various Ways (continued)

To obtain	From	Compute		
mole fraction	grams of solute per liter of solution	$n = \frac{G(MW_2)}{G(MW_2 - MW_1) + 1000 d(MW_1)}$		
weight percent of solute	mole fraction	wt % = $\frac{100 n(MW_1)}{n(MW_1) + MW_2(1 - n)}$		
weight percent of solute	grams of solute per liter of solution	$\text{wt } \% = \frac{G}{10 d}$		
weight percent of solute	molarity	$\text{wt } \% = \frac{M(\text{MW}_1)}{10 \ d}$		
weight percent of solute	molality	$\text{wt } \% = \frac{100 m(\text{MW}_1)}{1000 + m(\text{MW}_1)}$		
molality	molarity	$m = \frac{1000 M}{1000 d - M(\text{MW}_1)}$		
molality	grams of solute per liter of solution	$m = \frac{1000 G}{\text{MW}_1(1000 d - G)}$		
molality	weight percent of solute	$m = \frac{1000(\text{wt \%})}{\text{MW}_1(100 - \text{wt \%})}$		
molality	mole fraction	$m = \frac{1000 n}{\text{MW}_2 - n(\text{MW}_2)}$		

TABLE 11.6 Conversion Factors

The data have been compared with the *International Standard ISO* 31 (1979–80) and the *American Society for Testing and Materials Standard for Metric Practice E* 380-79. Relations which are exact are indicated by an asterisk (*). Factors in parentheses are also exact.

To convert	Into	Multiply by		
ampere per square centimeter ampere-hour ampere-turn	ampere per square inch* coulomb* gilbert meter*	6.4516 3600 1.256637 1×10 ⁻¹⁰		
apostib	nanometer* candela per square meter lambert*	0.1 0.3183099(1 π) 1×10 ⁻⁴		
atmosphere	bar* inch of mercury millimeters of mercury* millimeter of water newton per square meter* pascal* torr*	1.01325 29.92126 760 1.033227×10^{4} 1.01325×10^{5} 1.01325×10^{5} 760		

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TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by 0.986923 1×10 ⁶ 750.062 1×10 ⁵		
bar	atmosphere dyne per square centimeter* millimeter of mercury pascal			
barn	square meter*	1×10^{-28}		
barrel (petroleum)	gallon (British) gallon (U.S.)* liter	34.9723 42 158.987		
barrel (U.S., dry)	bushel (U.S.) liter	3.28122 115.6271		
barrel (U.S., liquid)	gallon (U.S.) liter	31.5 119.2405		
becquerel	curie*	2.7×10^{-11}		
British thermal unit (Btu)	calorie joule kilowatt-hour liter-atmosphere	251.996 1055.056 2.93071×10^{-4} 10.4126		
bushel (U.S.)	barrel (U.S., dry) cubic foot cubic inch* gallon (U.S.) liter pint (U.S., dry) quart (U.S., dry)	0.304765 1.244456 2150.42 9.30918 3.523907 64		
calorie	Btu joule* liter-atmosphere	0.003 968 320 4.186 8 0.041 320 5		
calorie (thermochemical)	joule*	4.184		
calorie per minute	watt*	0.06978		
calorie per second	watt*	4.1868		
candela	Hefner unit lumen per steradian*	1.11 1		
candela per square centimeter	candela per square foot* lambert	929.303 4 3.141 593(π)		
carat (metric)	gram*	0.2		
Celsius (Centigrade) temperature scale, °C	Fahrenheit temperature scale, °F	$\frac{9}{5}$ (°C + 32) = °F		
centimeter	foot inch mil	0.0328084 0.3937008 393.7008		
centimeter of mercury	pascal	1333.22		
centimeter per second	foot per second	0.0328084		

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by	
centimeter-dyne	erg* joule*	1 1×10 ⁻⁷	
centipoise	pascal-second*	0.001	
centistokes	square meter per second*	1×10^{-6}	
coulomb	ampere-second*	1	
cubic centimeter	cubic foot liter* ounce (U.S., fluid) quart (U.S., dry) quart (U.S., liquid)	3.53147×10^{-5} 0.001 0.03381402 9.08083×10^{-4} 0.001056688	
cubic centimeter per second	liter per hour*	3.6	
curie	becquerel*	3.7×10^{10}	
cycle per second	hertz*	1	
day (mean solar)	hour* minute* second	24 1 440 8.64 × 10 ⁴	
Debye unit	coulomb-meter	3.33564×10^{-30}	
decibel	neper	0.115 129 255	
degree (angle)	circumference minute (angle)* quadrant radian	0.00277778(1/360) 60 0.0111111(1/90) 0.01745329(π/180)	
degree Celcius (Centigrade) (temperature difference), °C	degree Fahrenheit, °F* degree Rankine* kelvin*	1.8 1.8 1	
dram (apothecaries or troy)	dram (avoirdupois)	2.1942857	
dram (avoirdupois)	grain* gram ounce (avoirdupois)	27.34375 1.7718452 0.0625(1/16)	
dram (U.S., fluid)	cubic centimeter ounce (U.S., fluid)* pint (U.S., liquid)*	3.696 691 2 0.125(1/8) 0.007 812 5(1/128)	
dyne	kilogram-force newton*	$1.019716 \times 10^{-6} \\ 1 \times 10^{-5}$	
dyne per square centimeter	bar* millimeter of mercury pascal	$ \begin{array}{r} 1 \times 10^{-6} \\ 7.500617 \times 10^{-4} \\ 0.1 \end{array} $	
dyne-centimeter	erg* joule* newton-meter*	$ \begin{array}{c} 1 \\ 1 \times 10^{-7} \\ 1 \times 10^{-7} \end{array} $	

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TABLE 11.6 Conversion Factors (continued)

To convert	Into	Multiply by
dyne-second per square centimeter	poise* pascal-second	1 0.1
electronvolt	erg	1.60219×10^{-12} 1.60219×10^{-19}
em	joule millimeter	4.217.52
erg	dyne-centimeter* joule* watt-hour	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Fahrenheit temperature, °F	Celsius temperature, °C	$\frac{5}{9}(^{\circ}F - 32) = ^{\circ}C$
fathom	foot*	6
fermi	meter*	1×10^{-15}
foot	centimeter* inch	30.48 12
foot-candle	lumen per square foot* lumen per square meter	1 10.7639
foot-lambert	candela per square centimeter candela per square foot lambert	3.42626×10^{-4} 0.3183099 0.00107639
gallon (British, imperial)	gallon (U.S.) liter*	1.20095 4.54609
gallon (U.S.)	liter ounce (U.S., fluid)* pint (U.S., liquid)*	3.785412 128 8
gauss	tesla* weber per square meter	$1 \times 10^{-4} \\ 1 \times 10^{-4}$
gilbert	ampere-turn	0.795775
grain	milligram*	64.79891
gram	carat (metric)* grain ounce (avoirdupois) ounce (troy) pound ton (metric)	$\begin{array}{c} 5 \\ 15.432358 \\ 0.035273962 \\ 0.032150747 \\ 0.0022046226 \\ 1 \times 10^{-6} \end{array}$
gram-force	dyne* newton*	980.665 0.009 806 65
gram-force per square centimeter	pascal*	98.0665
gram-force-centimeter	joule*	9.80665×10^{-5}
Hefner unit	candela	0.9
hertz	cycles per second*	1

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by		
hour (mean solar)	minute* second	60 3 600		
inch	centimeter* foot mil* millimeter*	2.54 0.083 333 3(1/12) 1 000 25.4		
joule	Btu calorie erg* liter-atmosphere newton-meter* watt-hour	9.478170×10^{-4} 0.2388459 1×10^{7} 0.009869233 1 $2.77778 \times 10^{-4}(1/3600)$		
kelvin temperature scale, K	Celsius scale, °C	$^{\circ}$ C + 273.1 = K		
kilocalorie per second	kilowatt*	4.1868		
kilogram	ounce (avoirdupois) ounce (troy) pound ton (long) ton (metric) ton (short)	$\begin{array}{c} 35.273963 \\ 32.150747 \\ 2.2046226 \\ 9.8420653\times10^{-4} \\ 0.001 \\ 0.0011023113 \end{array}$		
kilometer	foot light-year mile (statute)	3280.840 1.05702×10^{-13} 0.621371192		
kilowatt	Btu per hour horsepower (metric) joule per hour* kilocalorie per hour	3412.14 1.35962 3.6×10^{-6} 859.845		
knot	foot per minute meter per minute mile (nautical) per hour* mile (statute) per hour	101.2686 30.8667 1 1.15078		
lambert	candela per square centimeter	0.318310		
liter	cubic centimeter* cubic decimeter* cubic inch gallon (U.S.) ounce (U.S., fluid) pint (U.S., liquid) quart (U.S., liquid)	1 000 1 61.02374 0.2641721 33.81402 2.113376 1.056688		
liter per minute	gallon (U.S.) per hour	15.8503		
liter-atmosphere	Btu calorie joule*	0.0960376 24.2011 101.325		

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TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by		
lumen per square centimeter	lux*	1×10^{4}		
lux	lumen per square meter*	1		
maxwell	weber*	1×10^{-8}		
megaohm	ohm*	1×10^{6}		
meter	angstrom* foot	$ \begin{array}{c} 1 \times 10^{10} \\ 3.280839895 \end{array} $		
mho (ohm ⁻¹)	siemens*	1		
micrometer (micron)	angstrom millimeter*	1×10^4 0.001		
mil	inch* millimeter*	0.001 0.0254		
mile (statute)	foot* furlong* kilometer* mile (nautical)	5.280 8 1.609344 0.868976		
milligram per assay ton	milligram per kilogram ounce (troy) per ton (short)*	34.285714 1		
milliliter	cubic centimeter*	1		
millimeter	inch	0.0393708		
millimeter of mercury	atmosphere dyne per square centimeter pascal torr*	0.001315789(1/760) 1333.224 133.3224		
minute (angle)	circumference degree (angle) radian second (angle)*	$\begin{array}{c} 4.62963 \times 10^{-5} \\ 0.0166667(1/60) \\ 2.90888 \times 10^{-4} \\ 60 \end{array}$		
minute	day hour second*	6.944444×10 ⁻⁴ 0.0166667(1/60) 60		
newton	dyne*	1×10^{5}		
newton per square centimeter	pascal*	1×10^4		
oersted	ampere per meter	79.577 5		
ounce (avoirdupois)	dram* grain* gram* ounce (troy) pound*	16 437.5 28.349 523 125 0.911 458 33 0.062 5(1/16)		
ounce (U.S., fluid)	cubic centimeter gallon (U.S.)* milliliter	29.573 530 0.007 812 5(1/128) 29.573 530		

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by
	pint (U.S., liquid)* quart (U.S., liquid)*	0.0625(1/16) 0.03125(1/32)
parsec	kilometer	3.08568×10^{13}
part per million	gram per ton (metric)* milligram per kilogram*	1 1
pascal	bar* dyne per square centimeter* inch of mercury millimeter of mercury newton per square meter*	$ \begin{array}{c} 1 \times 10^{-5} \\ 10 \\ 2.95300 \times 19^{-4} \\ 7.50062 \times 10^{-3} \\ 1 \end{array} $
pascal-second	poise*	10
pica (printer's)	point*	12
pint (U.S., liquid)	cubic centimeter	473.1765
point (printer's, U.S.)	millimeter*	0.3514598
poise	pascal-second*	0.1
pound	dram* grain* gram* ounce (avoirdupois)* ton (long) ton (metric)* ton (short)*	256 7000 453.59237 16 4.4622857×10^{-4} 4.5359237×10^{-4} $5 \times 10^{-4} (1/2000)$
poundal	gram-force newton	14.098 1 0.138 255
proof (U.S.)	percent alcohol by volume*	0.5
quart (U.S., dry)	cubic centimeter cubic foot pint (U.S., dry)	1101.221 0.038 889 25 2
quart (U.S., liquid)	gallon (U.S.)* liter ounce (U.S., fluid)* pint (U.S., liquid)*	0.25 0.946353 32 2
radian	degree (angle) minute (angle) revolution	57.295 780 3.437.75 0.159 155
ream	quire* sheet	20 480 or 500
revolution	degree (angle)*	360
revolution per minute	radian per second	0.140720
roentgen	coulomb per kilogram*	2.58×10^{-4}
second (angle)	degree radian	2.77778×10^{-4} 4.848137×10^{-6}

11.14 SECTION 11

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by		
siemens	mho (ohm ⁻¹)*	1		
steradian	sphere spherical right angle	0.079 577 5 0.636 620		
stokes	square meter per second*	1×10^{-4}		
tablespoon (metric)	cubic centimeter*	15		
teaspoon (metric)	cubic centimeter*	5		
tesla	weber per square meter*	1		
ton (long)	kilogram* pound* ton (metric) ton (short)*	1016.0469088 2240 1.0160469 1.12		
torr	millimeter of mercury pascal	1 133.3224		
volt-second	weber*	1		
watt	Btu per hour calorie per second erg per second* joule per second*	3.41214 0.238846 1 × 107 1		
weber	maxwell*	1×10^{8}		
X unit	meter	1.00202×10^{-13}		

STATISTICS

TABLE 11.7 Values of t

df	t _{.60}	t.70	t _{.80}	t _{.90}	t _{.95}	t _{.975}	t _{.99}	t _{.995}
1	0.325	0.727	1.376	3.078	6.314	12.706	31.821	63.657
2	0.289	0.617	1.061	1.886	2.920	4.303	6.965	9.925
3	0.277	0.584	0.978	1.638	2.353	3.182	4.541	5.841
4	0.271	0.569	0.941	1.533	2.132	2.776	3.747	4.604
5	0.267	0.559	0.920	1.476	2.015	2.571	3.365	4.032
6	0.265	0.553	0.906	1.440	1.943	2.447	3.143	3.707
7	0.263	0.549	0.896	1.415	1.895	2.365	2.998	3.499
8	0.262	0.546	0.889	1.397	1.860	2.306	2.896	3.355
9	0.261	0.543	0.883	1.383	1.833	2.262	2.821	3.250
10	0.260	0.542	0.879	1.372	1.812	2.228	2.764	3.169

TABLE 11.7 Values of *t* (*continued*)

			1	1	1	1		
df	t _{.60}	t _{.70}	t _{.80}	t _{.90}	t.95	t _{.975}	t _{.99}	t _{.995}
11	0.260	0.540	0.876	1.363	1.796	2.201	2.718	3.106
12	0.259	0.539	0.873	1.356	1.782	2.179	2.681	3.055
13	0.259	0.538	0.870	1.350	1.771	2.160	2.650	3.012
14	0.258	0.537	0.868	1.345	1.761	2.145	2.624	2.977
15	0.258	0.536	0.866	1.341	1.753	2.131	2.602	2.947
16	0.258	0.535	0.865	1.337	1.746	2.120	2.583	2.921
17	0.257	0.534	0.863	1.333	1.740	2.110	2.567	2.898
18	0.257	0.534	0.862	1.330	1.734	2.101	2.552	2.878
19	0.257	0.533	0.861	1.328	1.729	2.093	2.539	2.861
20	0.257	0.533	0.860	1.325	1.725	2.086	2.528	2.845
21	0.257	0.532	0.859	1.323	1.721	2.080	2.518	2.831
22	0.256	0.532	0.858	1.321	1.717	2.074	2.508	2.819
23	0.256	0.532	0.858	1.319	1.714	2.069	2.500	2.807
24	0.256	0.531	0.857	1.318	1.711	2.064	2.492	2.797
25	0.256	0.531	0.856	1.316	1.708	2.060	2.485	2.787
26	0.256	0.531	0.856	1.315	1.706	2.056	2.479	2.799
27	0.256	0.531	0.855	1.314	1.703	2.052	2.473	2.771
28	0.256	0.530	0.855	1.313	1.701	2.048	2.467	2.763
29	0.256	0.530	0.854	1.311	1.699	2.045	2.462	2.756
30	0.256	0.530	0.854	1.310	1.697	2.042	2.457	2.750
40	0.255	0.529	0.851	1.303	1.684	2.021	2.423	2.704
60	0.254	0.527	0.848	1.296	1.671	2.000	2.390	2.660
120	0.254	0.526	0.845	1.289	1.658	1.980	2.358	2.617
∞	0.253	0.524	0.842	1.282	1.645	1.960	2.326	2.576
df*	-t _{.40}	-t _{.30}	-t _{.20}	-t _{.10}	-t _{.05}	$-t_{.025}$	-t _{.01}	-t _{.006}

^{*}When the table is read from the foot, the table values should be prefixed with a negative sign. Interpolation should be performed using the reciprocals of the degrees of freedom.

Source: Perry, Chilton, and Kirkpatrick, Chemical Engineers' Handbook, 4th ed., McGraw-Hill, New York (1963).

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